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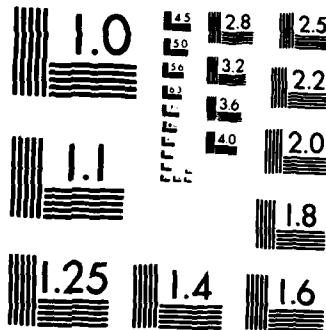
SSBAUER SPECTROMETRY: TESTING OF A NEW
COMPUTER BASED SYSTEM AND ITS
APPLICATION TO A STUDY OF AN
ALUMINUM-IRON-CERIUM ALLOY

THESIS

Joseph F. Harmon Jr.
Second Lieutenant, USAF
AFIT/GNE/PH/84M-6

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DEPARTMENT OF THE AIR FORCE

AIR UNIVERSITY (ATC)

# AIR FORCE INSTITUTE OF TECHNOLOGY

Wright-Patterson Air Force Base, Ohio

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ALUMINUM-IRON-CERIUM ALLOY


THESIS


Presented to the Faculty of the School of Engineering of

the Air Force Institute of Technology Air University In

Partial Fulfillment of the Requirements for the Degree of

Master of Science



by

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Second Lieutenant, USAF

Graduate Nuclear Engineering

March 1984

## Preface

This thesis is the product of my efforts to interface a new Mossbauer spectrometer to a PDP 11/03 microcomputer, which has the capabilities of analyzing Mossbauer data, and also to determine microstructure changes of an Al-Fe-Ce alloy due to various processing stages. This thesis will describe both the hardware and software changes made to assemble the new system, the system's limitations, and a complete operating procedure. For the alloy studied, a literature review and spectra for each processing stage is included.

I would like to thank Don Elworth of the Physics Department for his technical assistance throughout the project, and Doug Barker of the Air Force Materials Laboratory for supplying the alloy samples. I especially want to thank my advisor, Dr. George John, for his continuous support and guidance during this project.

Finally, I want to thank my wife, Rosie, for her constant support and understanding.

Joseph F. Harmon Jr.

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## Abstract

In this study, a computer based Mossbauer spectrometer was built using a new MS-900 spectrometer, an APPLE 2+ computer system, and a PDP 11/03 computer system. The APPLE was used as the link between the spectrometer and the PDP, which is used to analyze the Mossbauer spectra. In addition to minor hardware connections, software changes were made to the analysis program so that it could accept the data format produced by the new spectrometer. Due to equipment failure, only preliminary tests were made of the new system, however the tests were positive. Originally, an Al-Fe-Ce alloy was chosen to be studied by the new system. Instead, the alloy, chosen because of its excellent high temperature properties, was studied by the original Mossbauer spectrometer system. The goal was to follow and identify changes in the microstructure of the alloy due to different processing stages. Although changes in the spectra were identified with processing stages, it is still unclear as to what compounds are related to the observed spectra.

MOSSBAUER SPECTROMETRY: TESTING OF A NEW COMPUTER BASED SYSTEM

AND ITS APPLICATION TO A STUDY OF AN ALUMINUM-IRON-CERIUM ALLOY

## I.    Introduction

Mossbauer spectrometry is becoming an increasingly important tool for the field of physical metallurgy. The goal of this study consisted of assembling and testing a computer based mossbauer spectrometer and its application to examining an alloy consisting of 88% Al, 8% Fe, and 4% Ce by weight. This alloy was chosen to be studied by the Air Force Materials Laboratory because of its attractive elevated temperature and creep resistance properties.

## Background

In previous years, students have studied mossbauer spectrometry and its application to materials technology. These studies included: 1) the monitoring of chemical changes which occur during the manufacture of rare earth-cobalt magnets, 2) the determination of chemical changes in the bonding surface between a coating and its substate, and 3) the physical characteristics of amorphous metallic materials. The equipment used for these studies, including the software for data analysis, involved tedious manual transfer of data to a computer. In 1981 Pate succesfully completed the programing for a DEC LSI-11/03 computer which permits rapid analysis of mossbauer spectra without the need for a central processor at

The Air Force Institute of Technology. With this completed, it was desired to replace the aging and bulky spectrometer with a new one which could be interfaced with the DEC, resulting in rapid easy collection and analysis of data.

The alloy to be studied and used as a test for the newly built system was chosen by the Materials Laboratory at Wright Patterson Air Force Base. This organization has been involved in the study of powder metallurgy aluminum base alloys in order to improve elevated temperature strength and creep resistance properties. Initially, a total of 21 binary and ternary alloys fabricated from atomized powders, hot pressed to full density, were chosen to evaluate the effect of alloy composition and fabrication parameters on mechanical properties up to 405 - 650 F. From this study, the Al-Fe-Ce alloy was most promising and demonstrated that powder metallurgy was feasible for producing a new generation of elevated temperature aluminum alloys. However, it is still unclear as to the exact mechanism surrounding Ce. Also, it is realized that the type of processing will definitely influence the final product. Thus it is desirable to better understand the microstructure and how the microstructure is affected by changes in the processing parameters.

## Problem

The problem investigated in this study was twofold. First, an interface between the new spectrometer and the DEC was to be accomplished. Second, the new system was to be used for

studying the aluminum-iron-cerium alloy. In particular, the
alloy was to be analyzed at each stage of processing to follow
and identify changes in the microstructure. The processing
stages include: 1) gas atomization, 2) cold isostatic pressing,
3) hot vacuum degassing, and 4) hot isostatic pressing followed
by hot vacuum degassing.

## Scope

The interfacing achieved in this study was only a
temporary solution. Instead of a direct link between the new
spectrometer and the DEC, an APPLE 2 Plus computer was used to
link the two devices. Appendix B contains a brief discussion of
how a direct interface could be accomplished. Also, due to
equipment failure, the alloy tests had to be accomplished on the
original equipment. However, it was possible to test the new
equipment using a known source. In addition to these
limitations, the testing of all samples was taken at room
temperature and all samples were fabricated based on theoretical
calculations to optimize the spectra obtained. A literature
search was done and included sources at the Air Force Institute
of Technology, School of Engineering, an Air Force Wright
Aeronautical Laboratories technical report and a search by the
Mossbauer Effect Data Center in North Carolina on binary and
ternary alloys containing Al, Fe, and Ce.

## Review of the Literature

The literature review contains information found

pertaining to the Al-Fe-Ce alloy and the possible intermetallic compounds formed. Most of this information comes from the Air Force Materials Laboratory Technical Report. In order to better understand their results, it is necessary to explain how the test alloy was fabricated. First, the alloying elements Ce and Fe were added to 99.5% pure superheated aluminum and the alloy was then gas atomized in a low-oxygen flue gas to generate a fine, irregular powder (1:3). The low-oxygen flue gas was necessary to prevent violent oxidation (1:3). Following atomization, the powder was screened through a 325 mesh sieve and cold compacted at 414 MPa (60 Ksi) to form compacts with a density of about 80% of theoretical (1:4,47). Next, the compacts were heated to temperature in argon, transferred in air to a die and hot pressed to 100% density at 600 F or 700 F (1:48). Finally, the fully dense hot compacted billets were machined into forging preforms and hot forged at 600 F or 700 F.

The study by the Air Force Materials Laboratory indicated that this and the other alloys considered were likely to produce unknown metastable compounds due to the rapid solidification resulting from atomization. In order to try and identify the metastable intermetallic phases in the alloy, X-ray and thermal analysis, as well as optical metallography and scanning transmission electron microscopy (STEM), were used to study both the atomized powders and the forgings. Guinier-deWolf X-ray analysis revealed small amounts of $FeAl_6$ and an unidentified phase. The same structure was seen in both the powder and the forging samples (1:55). Thermal analysis,

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differential scanning calorimetry (DSC), also showed a lack of structural differences between the forgings upset at 600 F and 700 F and the atomized powders. Optical metallography revealed a very fine and uniform microstructure (1:11). Within a single particle, areas of fine, dense precipitates were interspersed with areas that appeared almost featureless at magnifications up to 1000X (1:103). It is believed that the featureless areas impart high strength while the precipitated areas contribute to increased ductility (1:164). In further efforts to identify the precipitated intermetallic phases present, a foil of the alloy was examined by STEM. The results indicated that some areas contain no Fe or Ce in the matrix while the intermetallics contained 90.5 at.% Al, 7.4 at.% Fe and 2.0 at.% Ce (1:103). These results however do not correspond to either of the ternary phases $Al_8 Ce Fe_4$ and $Al_{10} Fe_2 Ce$ stated to be possible formations in Al-Fe-Ce alloys (1:55).

When searching for information on ternary phases containing Al, Fe and Ce, only one other study was found. The study by Felner and Nowik shows Mossbauer spectra of an Fe57 probe replacing the Cu ion in the compound $Ce Cu_4 Al_8$ (2:1040). Their spectra, taken at temperatures from -452.29 F to room temperature, show a single quadrupole doublet with an isomer shift of +0.23 mm/s relative to Fe metal.

Finally, the most likely binary compounds formed, from the ratio of elements present, include Fe Al , Fe $Al_3$, Fe $Al_6$, $Fe_4 Al_{13}$ (3:299), and $Fe_2 Ce$ (4). Of these compounds, only information on Fe $Al_6$, $Fe_4 Al_{13}$, and $Fe_2 Ce$ was found. The spectra

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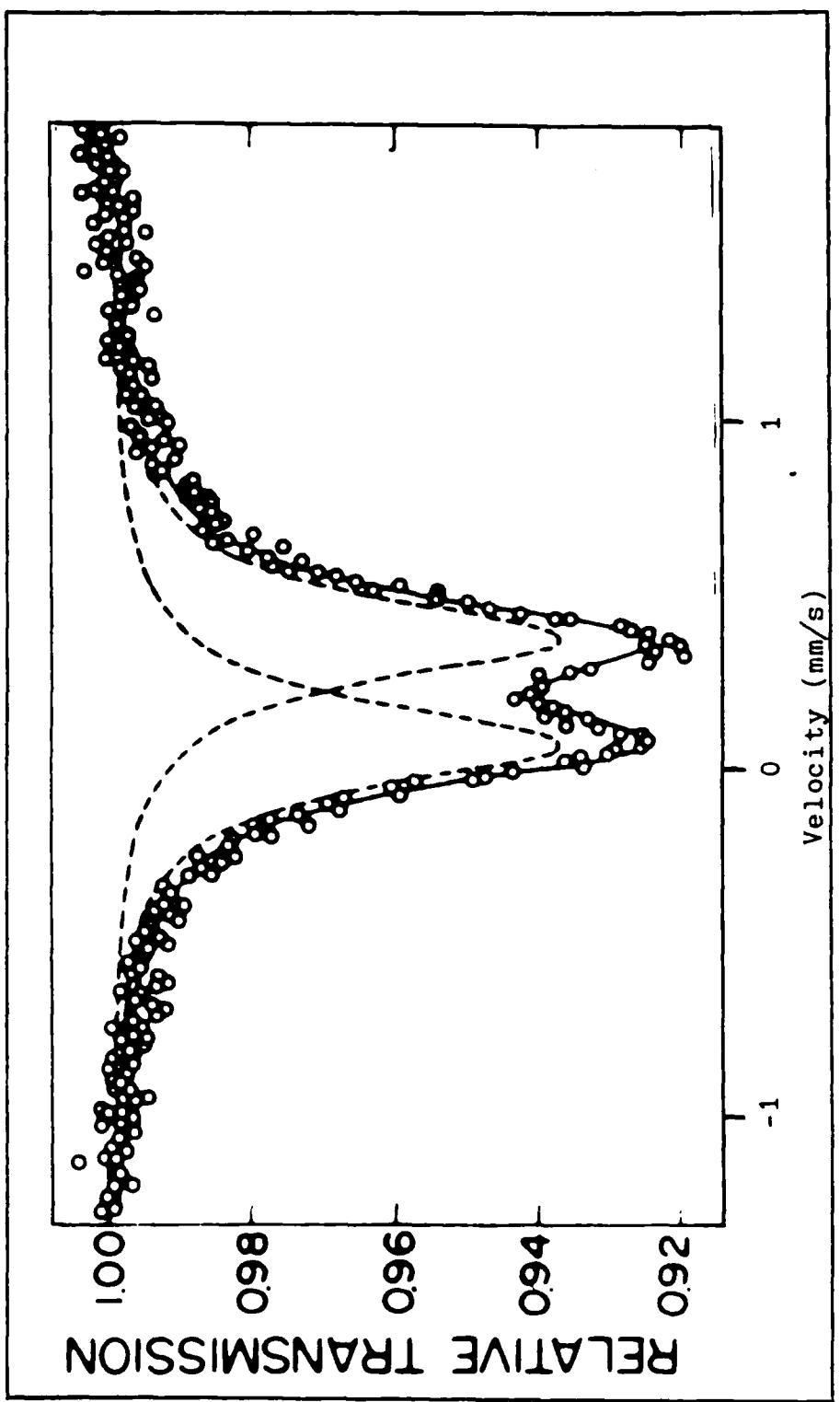
Figure 1. Spectra of FeAl$_6$ with respect to NFE.

or $Fe Al_6$ (Figure 1) is that of a quadrupole doublet with an isomer shift of +0.25 mm/s with respect to natural iron (3:301). The $Fe_4 Al_{13}$ spectra is the result of five different quadrupole doublets representing five different iron sites (5:1521). This spectra appears as a closely spaced triplet centered at 0.2 mm/s relative to natural iron foil (5:1522). The $Ce Fe_2$ spectra is a symmetric six line pattern and the curie temperature for this compound is reported to be -32.8 F (4:762).

## II. Theory

### Mossbauer Effect

The theory of the Mossbauer Effect has been well developed and thus will not be covered here in detail. For a detailed discussion the reader is referred to reference 6. Instead, a general description of the Mossbauer Effect will be given through the following example. Consider a nucleus of an atom bound in some type of lattice such as is the case of a metal. The nucleus may interact with its environment in three ways. First, the nuclear charge may interact electrostatically with the electrons present at the nucleus. A change in the electron density at the nucleus, from perhaps a change in the lattice structure, results in a shift of the nuclear energy levels. Second, the nuclear quadrupole moment of a nucleus can interact with an electric field gradient which is usually a result of the charge distribution of the ions in the lattice. An interaction of this type will cause splitting of the nuclear energy levels. For the case of an iron nucleus, the splitting will result in two nuclear energy levels. Finally, the magnetic dipole moment of a nucleus can interact with a magnetic field produced externally or due to ions in the lattice. This interaction also causes splitting of nuclear energy levels and for the case of an iron nucleus, six energy levels are produced.

In 1957, Rudolph Mossbauer noticed that by moving a radioactive source, the energy of a photon emitted by the nucleus was changed by a small amount. Mossbauer spectrometry takes advantage of this fact by using photons of a spectrum of

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energies, produced by accelerating a radioactive source, to probe the nuclear energy levels of a nucleus in its lattice. If the emitted photon, from a source, has the correct energy needed to excite the nucleus in a lattice, or absorber, then the photon may be absorbed and re-emitted isotropically resulting in a resonant effect. This effect will take place if the source and absorber both contain the same atom. Commonly, the source contains iron in an excited state and the absorber contains iron in the ground state. If the absorber is placed between the velocity modulated source and a detector, a spectrum containing dips, or lines, will be seen where each dip is a result of the resonant absorption. Each dip is related to a particular source velocity, and thus a particular photon energy, which is characteristic of the absorbing nuclei. From studying these spectra, a great deal can be learned about the environment of the iron nucleus. In this study, the alloy being tested contains an iron nucleus which will be used as a probe to uncover information about the alloy's lattice structure.

Absorber Parameters

A Mossbauer spectrum can be optimized by choosing the proper absorber thickness. A method by Shimony (7) enables one to find the best absorber thickness for maximizing the relative intensity of the absoption lines. This method is based on maximizing a single line, but can be extended to cases where there are several lines of equal intensity (7:350).

If an absorber is made very thick, there will be a

large number of active nuclei in the path of an incident photon, resulting in a strong resonant effect. However, if the absorber is too thick, the non-resonant radiation emerging from the absorber will be very weak. Because of this, the resonance lines will appear very slowly due to statistics involved and the background noise will tend to mask it out (7:348). If the absorber is too thin, the emerging non-resonant beam will be increased but the resonance effect will be reduced because of fewer active nuclei present in the path of the incident photon. The method to be described below enables one to calculate an intermediate thickness which will result in maximum absorption peaks.

Initially, one assumes that the shape of the resonant line(s) is Lorentzian, which is true unless perturbed by the system (8:3,5). If this is the case, then the magnitude of the Lorentzian peaks, according to Shimony, can be expressed as (7:349):

$$q(d)=N_0 f_s(1-exp(-1/2u_r d)J_0(1/2iu_r d))exp(-u_a d) \qquad (1)$$

where,

d  = actual absorber thickness

$N_0$ = number of photons striking the absorber

$f_s$ = recoil free fraction of the source

$u_r$ = coefficient of resonant absorption

$u_a$ = coefficient of non-resonant absorption

$J_0$ = zero-order Bessel function

If equation (1) is examined closely, it is noticed that for $d = 0$ and as $d \rightarrow \infty$, $q(d)$ vanishes. By setting the derivative of $q(d)$ with respect to $d$ equal to zero and using the identity

$$(dJ_0(x))/dx = -J_1(x) \tag{2}$$

the following relation is found:

$$\frac{u_r}{2u_a} = \frac{(\exp(1/2u_r d_0) - J_0(1/2iu_r d_0))}{(J_0(1/2iu_r d_0) + J_1(1/2iu_r d_0))} \tag{3}$$

which yields Table 1 (7:349). If one can find the value of the dimensionless quantity $u_r/2u_a$, one can use table 1 to find the value of $1/2u_r d_0$ and thus $d_0$.

The value of $u_r$ can be found through the relation

$$u_r = f_a n s_0/M \tag{4}$$

where

$f_a$ = recoiless traction of the absorber

$n$ = number density of active nuclei in absorber

$M$ = number of equal intensity peaks

$s_0$ = maximum average cross section for resonant absorption per active nucleus

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Table 1.

$\frac{1}{2} u_r d_0$ as a Function of $u_r/(2u_a)$

| $\frac{1}{2} u_r d_0$ | $u_r/(2u_a)$ | $\frac{1}{2} u_r d_0$ | $u_r/(2u_a)$ | $\frac{1}{2} u_r d_0$ | $u_r/(2u_a)$ |
|---|---|---|---|---|---|
| 0.0 | 0.0000 | 2.2 | 8.946 | 5.8 | 53.83 |
| 0.1 | 0.1078 | 2.3 | 9.760 | 6.0 | 57.03 |
| 0.2 | 0.2324 | 2.4 | 10.620 | 6.2 | 60.33 |
| 0.3 | 0.3758 | 2.5 | 11.50 | 6.4 | 63.67 |
| 0.4 | 0.5397 | 2.6 | 12.42 | 6.6 | 67.02 |
| 0.5 | 0.7264 | 2.7 | 13.36 | 6.8 | 70.42 |
| 0.6 | 0.9379 | 2.8 | 14.36 | 7.0 | 73.94 |
| 0.7 | 1.176 | 2.9 | 15.36 | 7.2 | 77.47 |
| 0.8 | 1.445 | 3.0 | 16.40 | 7.4 | 81.05 |
| 0.9 | 1.741 | 3.2 | 18.55 | 7.6 | 84.73 |
| 1.0 | 2.072 | 3.4 | 20.79 | 7.8 | 88.46 |
| 1.1 | 2.433 | 3.6 | 23.13 | 8.0 | 92.18 |
| 1.2 | 2.837 | 3.8 | 25.55 | 8.2 | 95.87 |
| 1.3 | 3.276 | 4.0 | 28.06 | 8.4 | 100.1 |
| 1.4 | 3.749 | 4.2 | 30.78 | 8.6 | 103.8 |
| 1.5 | 4.261 | 4.4 | 33.39 | 8.8 | 107.9 |
| 1.6 | 4.839 | 4.6 | 36.05 | 9.0 | 113.3 |
| 1.7 | 5.404 | 4.8 | 38.87 | 9.2 | 115.9 |
| 1.8 | 6.039 | 5.0 | 41.71 | 9.4 | 120.6 |
| 1.9 | 6.703 | 5.2 | 44.65 | 9.6 | 124.6 |
| 2.0 | 7.416 | 5.4 | 47.62 | 9.8 | 128.7 |
| 2.1 | 8.160 | 5.6 | 50.72 | 10.0 | 132.5 |

For the alloy being studied, no data was available on the recoil free fraction. However, a value of 0.5 was assumed which is typical of many absorbers. For an iron atom, the value of $s_0$ is given as 2.38E-18 $cm^2$/Fe atom (9). The value for n was calculated to be 1.88E+19 atoms/g and from initial spectra, two peaks appeared with nearly equal intensities, thus a value of 2 will be given to M. These constants lead to a value of 11.208 $cm^2$/g for $u_r$.

The value for $u_a$ in $cm^2$/g was found by assuming the relation

$$u_{a_t} = \sum_i w_i u_{a_i} \qquad (5)$$

holds true (10:69). The values of each $u_a$ lead to a final value of 17.3 $cm^2$/g for the alloy. By using the values of $u_r$ and $u_a$ and table 1, a value of 0.047 $g/cm^2$ was calculated for the optimum absorber thickness. As will be shown later, this value differs from the experimentally found optimal value by approximately 50%. However, this method was useful for finding an initial value which was able to be refined experimentally.

## III. Equipment and Procedures

In this section, the Mossbauer spectrometry equipment and procedures for data aquisition will be discussed. The equipment for the original system will simply be listed while the equipment and installation procedure will be included for the new system. Also discussed will be the method of absorber preparation, the experimental method for finding the optimum absorber thickness, and the experimental geometry.

### Original Mossbauer System

The major components of the original Mossbauer spectrometer include a velocity transducer (motor), a motor control unit (MCU) to drive the motor at a constant acceleration, a linear amplifier/single channel analyzer, a Krypton-filled proportional counter with a preamplifier, and a high voltage supply for the detector. All of the above equipment, with exception for the detector, was manufactured by Ranger Electronics. Other equipment included a RIDL 400 multichannel analyzer (MCA) operated in a time-sequential scaling mode and driven by a RIDL time base oscillator.

### New Mossbauer System

The new Mossbauer spectrometer system consists of a single unit (MS-900) which contains the Mossbauer control unit, the linear amplifier/single channel analyzer, a time base oscillator and a 1024 multichannel analyzer. This unit, built by Ranger Scientific, Incorporated, was designed to be operated

with the assistance of an APPLE 2+ or 2e computer. Other
equipment used in conjunction with this unit included a velocity
transducer (VT-900) also built by Ranger Scientific,
Incorporated, a detector/preamplifier, and a high voltage
supply. In order to transfer and display data, an APPLE 2+
computer was connected to the MS-900 via an MS-900-100 interface
card inserted in the computer.

For both the new and original system, the operation is
basically the same. The source is connected to the shaft of the
velocity transducer, which is accelerated by the control unit.
This unit is driven by the channel address ramp from the
multichannel analyzer, which is driven by the time base
oscillator. The pulses produced by the detector are sent through
the preamplifier, linear amplifier and single channel analyzer
respectively. The single channel analyzer windows are set such
that only pulses resulting from the 14.4 kiloelectron volt (keV)
photons are passed through the remaining circuitry. As each
channel in the MCA is opened for a time specified by the time
base oscillator, pulses from the SCA enter this channel and thus
a spectrum of counts versus channel number is produced. Each
channel is related to a particular velocity of the source and
thus the spectrum is also that of counts versus velocity. How
the velocity scale is assigned to the spectrum during data
analysis will be discussed later. The velocity scale on this
spectrum depends on whether the motor is driven in the
triangular mode or flyback mode. In either case, the maximum
velocity (VMAX) of the source is set and the source is moved at

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a constant linear acceleration between +VMAX and -VMAX. For the flyback mode, the source velocity is varied from -VMAX to +VMAX and generates a single spectrum. For the triangular mode, the source velocity is varied from +VMAX to -VMAX and back to +VMAX. In this case, two identical spectra are seen. One spectrum is generated when accelerating from +VMAX to -VMAX and a mirror image spectra is generated when accelerating from -VMAX to +VMAX. Due to limitations in the data analysis program, to be discussed later, only the flyback mode was used in this study.

## Computer System

The computer system used for data analysis with both the new and original Mossbauer spectrometers consists of a PDP 11/03 microcomputer with 64 kilobytes of memory, an RX-02 dual 8-inch floppy disk drive, and a VT-100 terminal, all manufactured by Digital Equipment Corporation. Additionally, an MX-80 F/T dot matrix printer by Epson is serially connected to provide a printout of results.

The PDP 11/03 is a 16 bit word computer consisting of an LSI 11/02 microprocessor with a KEV-11 floating point chip, a BDV-11 bootstrap and diagnostic board, a DLV-11 4 port serial interface board, and a DRV-11 parallel interface board (8:9). All programming is in FORTRAN IV version 2.5 and all FORTRAN software was provided by Digital Equipment Corporation (8:9).

The computer system used for interfacing the MS-900 unit with the PDP 11/03 consists of an APPLE 2+ with 48 kilobytes of memory, an APPLE monitor III, 5 1/4-inch floppy

disk drive, and an APPLE Super Serial Card. Also, a joystick and
a Sylentype thermal printer was used for manipulating data and
printing results respectively. The software for data
manipulation was a Mossbauer Master program supplied by Ranger
Scientific, Incorporated for an APPLE 2+ or 2e computer. This
software enables one to do several things with the data
obtained. The options include acquiring data, storing data on a
disk, retrieving data from a disk, printing the data on a
printer, and displaying the spectrum. Changes made to this
software, as part of the new Mossbauer spectrometer
installation, are included in later sections.

## MOSFUN Program

Whether one is using the new or original spectrometer
system, the data must somehow be analyzed. The computer program
used for spectrum analysis in this study is MOSFUN, originally
written by E.W. Muller and modified by B.E. Pate in 1981 as a
thesis project. Pate modified the console version of MOSFUN,
designed to run on mainframe computers using terminals, to a
size and format which could fit into the PDP 11/03. By extensive
use of subroutines, an overlaying technique was able to be used
to fit the program into the smaller memory of the PDP 11/03. The
final version allows up to 32 fit parameters, 24 lines, and 1024
data points (8:15). The parameters used by MOSFUN to fit a
spectrum include intensity, position, half-width and possibly
form. These parameters are used in one of four possible models
provided by MOSFUN. Two models use Lorentzian lineshapes, one

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using line intensity and one using line area. The other two

models use Voigt lineshapes and again, one uses line intensity

and one uses line area. Only when using the Voigt theory is the

fourth parameter, form, used. This parameter determines whether

the lineshape is more Gaussian or Lorentzian.

There are two iterative methods, Newton and Gradient,

provided for correcting the initially calculated theoretical

spectrum in MOSFUN. Both are equally accurate. However, Newton's

method is much faster if it does not diverge. For this study,

the Lorentzian - intensity and Voigt-intensity theories were

used with the gradient method. Details of the parameters used

and theory applied to each spectra are discussed in chapter 4

(results/discussion). For a detailed description of the modified

MOSFUN program, the reader is referred to reference 8.

## New Spectrometer Insallation

In order to assemble a new system so that data could be

sent directly to the PDP 11/03 for anaylysis from the new

spectrometer, software and hardware changes had to be made. The

software changes included modifications made to both MOSFUN and

the Mossbauer Master program.

MOSFUN Changes . Basically, the changes made to MOSFUN

include altering the DATI and DRIVE subroutines to allow a 1024

data point spectrum with no velocity data included, instead of a

400 point spectrum with velocity data every 10 channels.

Additionally, the read statements for the time base data also

had to be changed. Originally, the first 14 channels contained

time base data and the remaining 386 channels contained Mossbauer data, with velocity data every ten channels, starting with channel 19. The new spectrometer does not contain a moire system and thus the spectrum contains no velocity data. The first two channels contain time base data while the remaining channels contain Mossbauer data. The first step taken was to allow subroutine DATI to accept the new spectrum format by reading in the first two data points as time base data, instead of the first 14. These points were then set equal to zero as originally done for the first 14 points. Next, a GOTO statement was added to bypass the velocity extraction portion of DATI. Normally, velocity points are stored in an array called VCON(I) and a linear least squares fit is done on the velocity data. Since the new system does not produce velocity data, the velocity values in mm/s and peak positions of a known spectrum were entered. The velocity values and channel positions for each peak of a natural iron spectrum were inserted into subroutine DATI. The velocity values, taken from reference 9, are those with respect to sodium nitroprusside. Thus, all spectra will be analyzed with respect to sodium nitroprusside. As before, a linear least squares fit will be done on the VCON(I) array and the channel numbers for each velocity point are set equal to zero. Finally, no changes had to be made to allow a 1024 point spectra instead of a 400 point one, because MOSFUN was originally equipped to handle this option.

The changes made to subroutine DRIVE include altering arrays X(I) and XY(I). Array X(I) contains the channel number

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corresponding to each velocity point and was originally assigned a value in subroutine DRIVE since velocity points were evenly spaced throughout the data. The array values are now assigned by entering them into subroutine DRIVE (see appendix A for procedure), where each channel number corresponds to a peak from the natural iron calibration run. Array XY(I) is an array containing values of VCON(I) which have been converted to mm/s. This conversion has been omitted since VCON(I) is entered as mm/s in subroutine DATI. The velocity values for each peak are from published calibration data and thus do not need to be changed. However, the channel locations for each peak, which must be entered into subroutines DRIVE and DATI, must be updated periodically to insure an accurately calibrated system. The present values are a result of a 25 micron thick natural iron absorber run at room temperature for 4.25 hours (figure 2).

   Mossbauer Master Changes . The changes made to the Mossbauer Master program permit data to be sent to the PDP 11/03, in addition to a printer or a disk. Also, once the hardware connections were made between the APPLE and the PDP, to be discussed later, the format in which the program transmitted or printed data had to be changed. Appendix C contains a listing of the Mossbauer Master program with the changes added. The format changes include using one line for the spectrum name, a second line for specifying the format in which MOSFUN reads the data, and a third line for listing the number of time base overflows, data overflows, number of data points total, number of data points in a full period, and the drive mode.
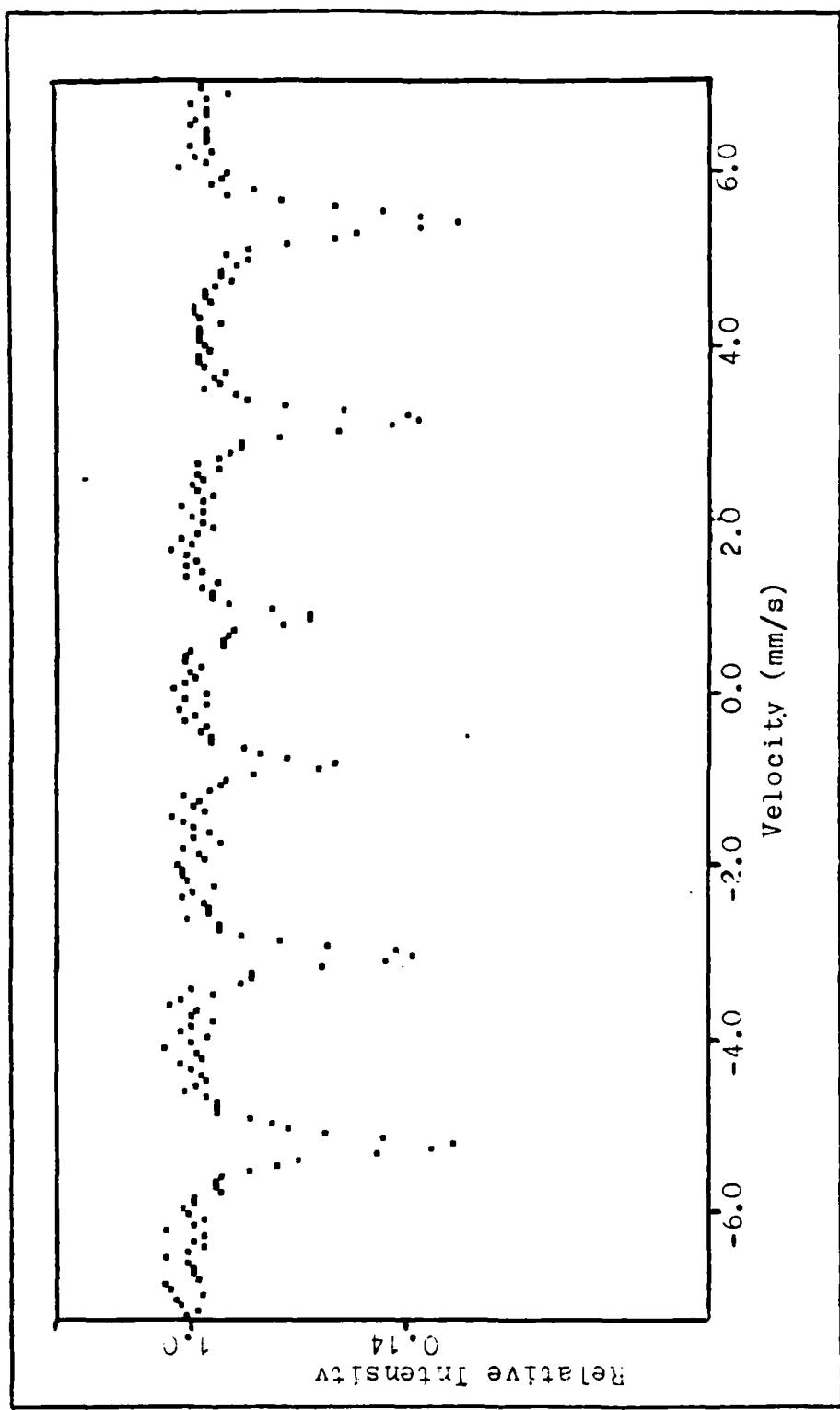
Fig 2. Natural Iron Calibration Results From MS-900
(With respect to Sodium Nitroprusside)

FE57TEST

```
Ø       14261 14261 3340 3434 3335 3382 2933 2407
8       3154 2957 2623 3231 2852 3148 2875 3036
16      3266 2593 2673 3199 3097 2151 3066 3336
24      3495 3393 3375 3315 3469 3545 3434 3391
32      3538 3400 3453 3444 3430 3469 3501 3465
40      3448 3479 3421 3457 3430 3424 3463 3462
48      3477 3472 3401 3474 3489 3484 3394 3540
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64      3442 3488 3381 3589 3528 3415 3417 3491
72      3356 3433 3323 3465 3474 3428 3350 3578
80      3404 3428 3342 3473 3492 3428 3462 3433
88      3458 3479 3471 3428 3499 3448 3314 3474
96      3428 3454 3483 3422 3334 3438 3389 3411
104     3504 3385 3322 3483 3428 3343 3350 3404
112     3421 3356 3348 3389 3396 3339 3418 3373
120     3288 3305 3379 3336 3374 3340 3266 3287
128     3377 3253 3323 3223 3304 3314 3372 3342
136     3419 3249 3347 3223 3226 3457 3268 3232
144     3346 3168 3180 3250 3162 3138 3228 3178
152     3256 3243 3209 3128 3159 3107 3082 3061
160     3186 2983 3021 2955 2983 2899 2970 2953
168     2852 2835 2689 2845 2661 2588 2615 2510
176     2470 2460 2358 2363 2186 2182 2103 2100
184     2108 1988 1926 2011 1881 1925 1908 1893
192     2030 1985 1975 2024 2033 2199 2136 2207
200     2439 2360 2360 2392 2448 2539 2563 2686
208     2816 2797 2843 2794 2850 2904 2944 2940
216     3069 3035 3063 3216 3171 3160 3204 3037
224     3178 3173 3082 3299 3134 3231 3242 3205
232     3214 3351 3290 3323 3198 3179 3332 3358
240     3303 3192 3302 3280 3227 3261 3286 3309
248     3314 3248 3248 3341 3319 3194 3305 3314
256     3345 3272 3357 3328 3229 3263 3242 3384
264     3347 3337 3316 3320 3200 3297 3310 3259
272     3368 3229 3199 3195 3166 3193 3319 3283
280     3306 3254 3193 3190 3216 3248 3296 3113
288     3109 3096 3048 3202 3076 3014 3117 3141
296     3071 3056 3011 2959 3084 2962 2987 2882
304     2947 2875 2760 2740 2731 2633 2582 2579
312     2563 2573 2426 2530 2381 2387 2238 2196
320     2108 2102 2034 2005 2038 1916 1876 1958
```

Figure 3. Old Data Format

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NFECAL.EX1
( 8F9.0)
0.0,1024,2048,3

| | | | | | |
|---|---|---|---|---|---|
| 89200 | 89200 | 14447 | 14200 | 14128 | 14457 | 14255 | 13091 |
| 14337 | 14412 | 13433 | 14315 | 14301 | 13872 | 14443 | 13843 |
| 14220 | 14578 | 13507 | 13989 | 14232 | 14095 | 13076 | 14087 |
| 14521 | 14302 | 14656 | 14412 | 14348 | 14175 | 14344 | 14342 |
| 14485 | 14357 | 14446 | 14509 | 14304 | 14374 | 14488 | 14313 |
| 14524 | 14476 | 14269 | 14369 | 14409 | 14484 | 14407 | 14462 |
| 14509 | 14670 | 14573 | 14608 | 14255 | 14479 | 14499 | 14659 |
| 14441 | 14530 | 14372 | 14351 | 14401 | 14107 | 14310 | 14428 |
| 14314 | 14328 | 14414 | 14627 | 14473 | 14472 | 14612 | 14585 |
| 14506 | 14332 | 14487 | 14537 | 14270 | 14531 | 14363 | 14356 |
| 14563 | 14421 | 14271 | 14434 | 14595 | 14438 | 14409 | 14584 |
| 14334 | 14384 | 14569 | 14317 | 14376 | 14555 | 14684 | 14503 |
| 14392 | 14293 | 14367 | 14299 | 14412 | 14396 | 14329 | 14386 |
| 14610 | 14420 | 14400 | 14451 | 14441 | 14447 | 14487 | 14240 |
| 14290 | 14516 | 14282 | 14449 | 14358 | 14384 | 14471 | 14396 |
| 14300 | 14187 | 14457 | 14474 | 14655 | 14474 | 14399 | 14131 |
| 14357 | 14273 | 14598 | 14344 | 14299 | 14260 | 14650 | 14362 |
| 14412 | 14405 | 14369 | 14428 | 14486 | 14385 | 14420 | 14476 |
| 14394 | 14465 | 14375 | 14309 | 14370 | 14533 | 14402 | 14309 |
| 14080 | 14236 | 14172 | 14143 | 14193 | 13973 | 14242 | 14262 |
| 14198 | 14115 | 14081 | 14201 | 14141 | 14162 | 13972 | 13853 |
| 13835 | 13849 | 13698 | 13622 | 13570 | 13516 | 13494 | 13314 |
| 13427 | 13135 | 13044 | 12732 | 12609 | 12607 | 12306 | 12054 |
| 12145 | 11995 | 12047 | 12239 | 11928 | 12205 | 12320 | 12441 |
| 12565 | 12650 | 12985 | 13036 | 13147 | 13488 | 13386 | 13627 |
| 13482 | 13664 | 13800 | 13688 | 13640 | 13864 | 13917 | 14024 |
| 13848 | 13921 | 14019 | 14031 | 14177 | 14156 | 14176 | 13849 |
| 14184 | 14171 | 14193 | 14130 | 14168 | 14186 | 14192 | 14240 |
| 14284 | 14420 | 14246 | 14389 | 14476 | 14341 | 14493 | 14285 |

Figure 4. New Data Format

23
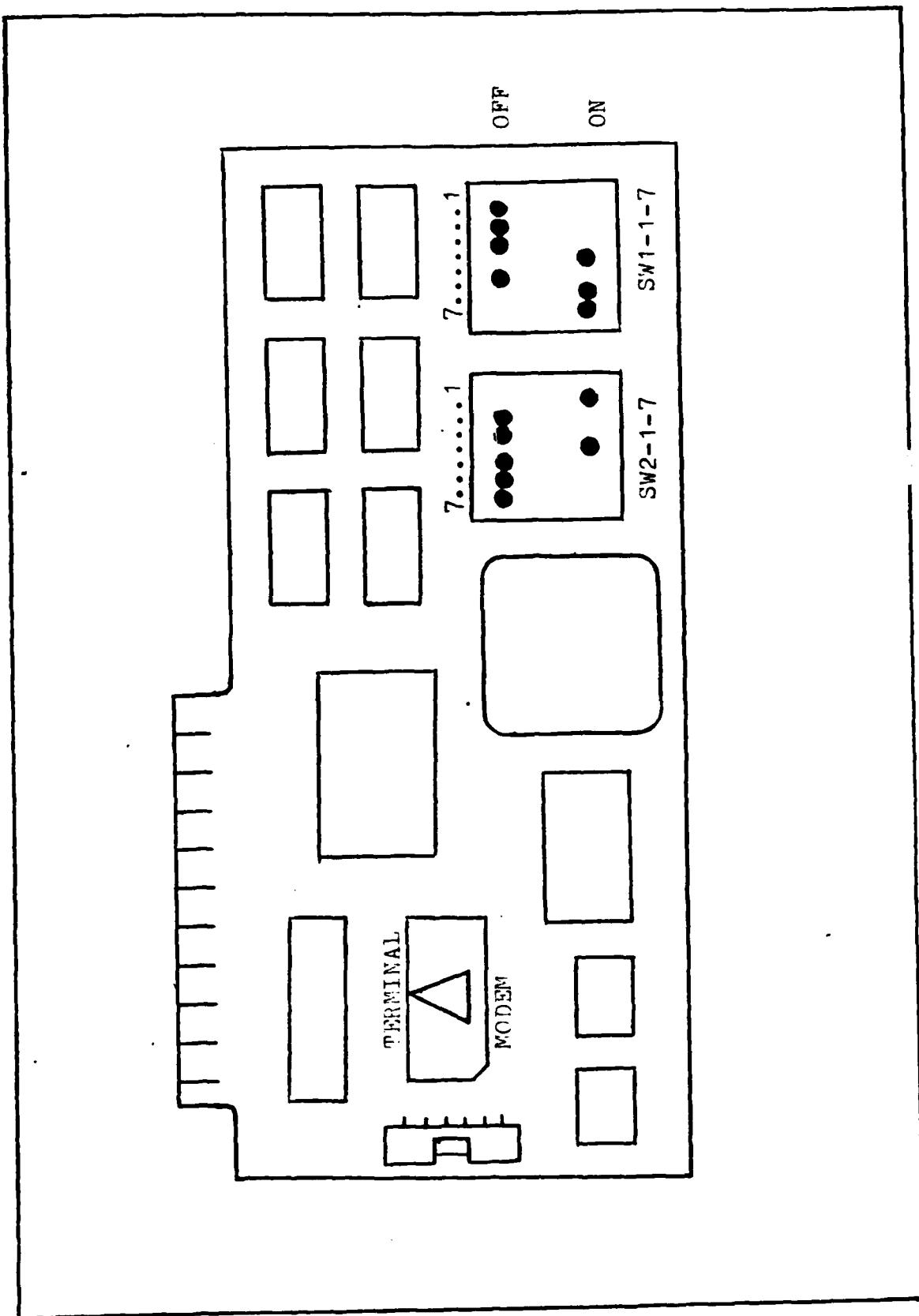
FIGURE 5. Super Serial Card Settings

Additionally, the data was made to be listed in an 8F9.0 format. In other words, there are 8 values per row with each value containing up to 9 characters. All of the changes mentioned above were made to conform to the format MOSFUN expects. Examples of the original and new formats are shown in figures 3 and 4.

Hardware Changes . The connection between the APPLE 2+ and the PDP 11/03 was made with an APPLE Super Serial card and a modified 10 wire connector cable. The card was inserted into slot number two of the APPLE and a series of switches on the card were set to match the connecting device which, in this case, was the PDP. The switch settings, shown in figure 5, control the baud rate, number of stop bits, carriage return delay, line width, and linefeed. Switches SW1-1 through SW1-4 control the baud rate and were set for a value of 9600 to match the PDP. Switches SW1-5 and SW1-6 control the operating mode of which the printer mode was used. This mode is used when sending data to a printer, a terminal, or in this case, another computer without the use of a modem. The number of stop bits sent to signal the end of a character is controlled by SW2-1 and was set for one stop bit. The carriage return delay, controlled by SW2-2, was set equal to zero since the PDP can accept data much quicker than a printer, which normally needs a small delay. Switches SW2-3 and SW2-4 control the linewidth and were set to produce 80 characters per line. Switch SW2-5 controls linefeed generation and was set to not produce a linefeed since the PDP does this automatically. Switches SW2-6, SW2-7, and SW1-7 were

TABLE 2.

DB-25 Pin Connections For Connector Cable Exiting APPLE 2+

| 10-pin header | DB-25 connector | Signal Name |
|---|---|---|
| 1 | 1 | Frame Ground |
| 2 | 2 | Transmit Data |
| 3 | 3 | Recieve Data |
| 4 | 4 | Request To Send |
| 5 | 5 | Clear To Send |
| 6 | 6 | Data Set Ready |
| 7 | 19 | Secondary Clear To Send |
| 8 | 7 | Signal Ground |
| 9 | 20 | Data Terminal Ready |
| 10 | 8 | Data Carrier Detect |

DB-25

14                                        25

1                                        13
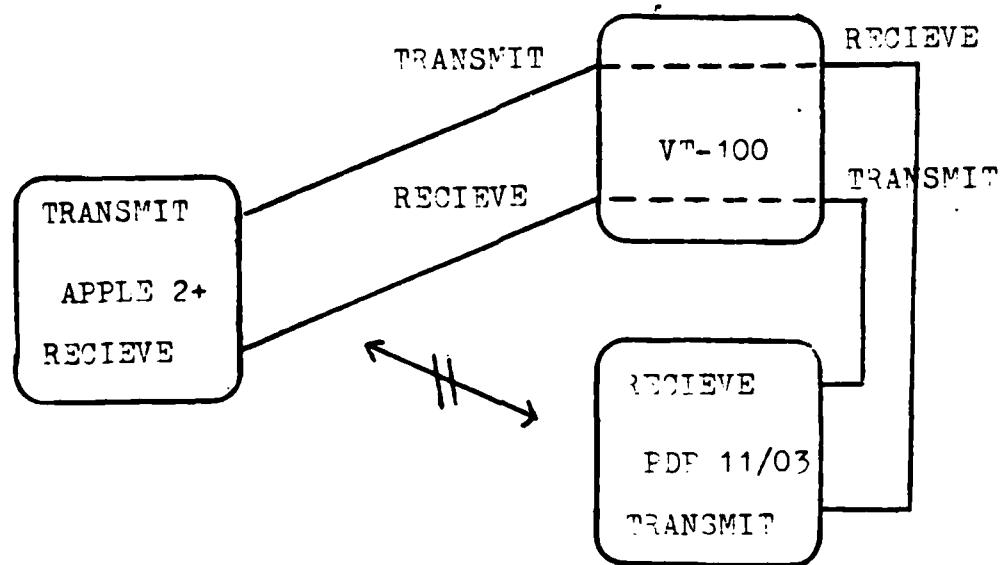
Data Transferred to VT-100 Only
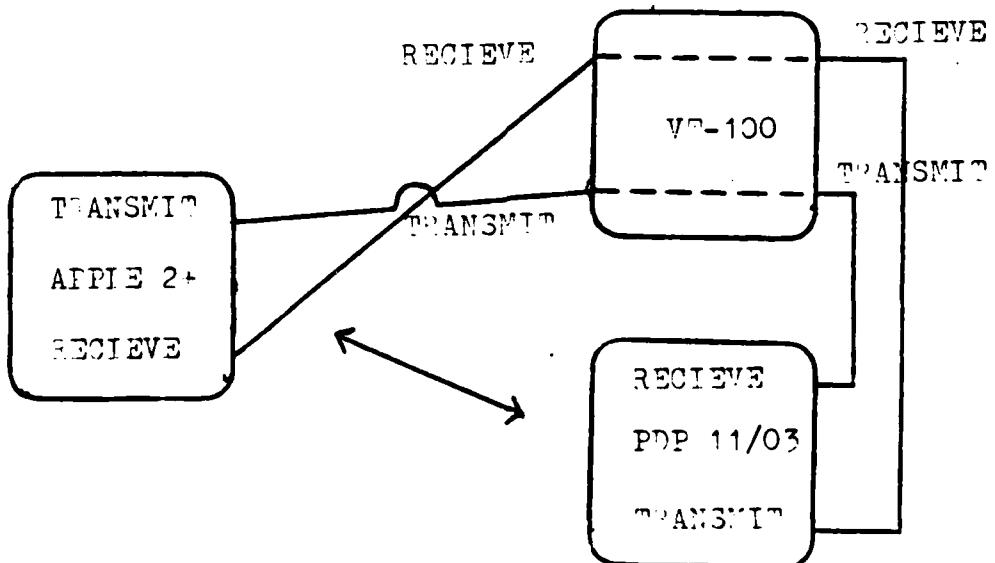
Data Transfered From APPLE 2+ To PDP 11/03 (Bypass VT-100)

FIGURE 6. Transmit/recieve Data Connection

set at the default settings specified by the card manual. These
switches are used for special cases and do not apply in this
situation. The only other adjustment made was to put the card
into printer, or terminal mode. This was accomplished by
extracting and reinserting the jumper block on the card such
that the triangle pointed towards terminal. This is also
illustrated in figure 5.

The connecting cable between the PDP and the Super
Serial card was the final step in the installation of the
system. A ten strand flat cable and two male DB-25 connectors
were used to make the connecting cable. The connector pin
assignments for the ten pin header on the card and the
corresponding pins on the DB-25 connector are shown in table 2.
The opposite end of the cable, which connects to the PDP, has
the same pin assignments except for the switching of pins two
and three. These connections are those for transmitting and
receiving data respectively. This switch is illustrated in
figure 6. In the printer or terminal mode, the transmit pin of
the Super Serial card is connected to the recieve pin of the
terminal and visa versa. This same relationship exists between
the PDP and the VT-100 terminal. Thus, in order for the APPLE to
communicate directly with the PDP, the transmit and recieve
cables were switched on one end of the connecting cable. The
connection to the PDP was made by disconnecting the female end
cable at the VT-100 terminal and reconnecting this end to the
male end of the modified connector cable mentioned above. Now,
data from the APPLE can be sent directly to the PDP to be put on

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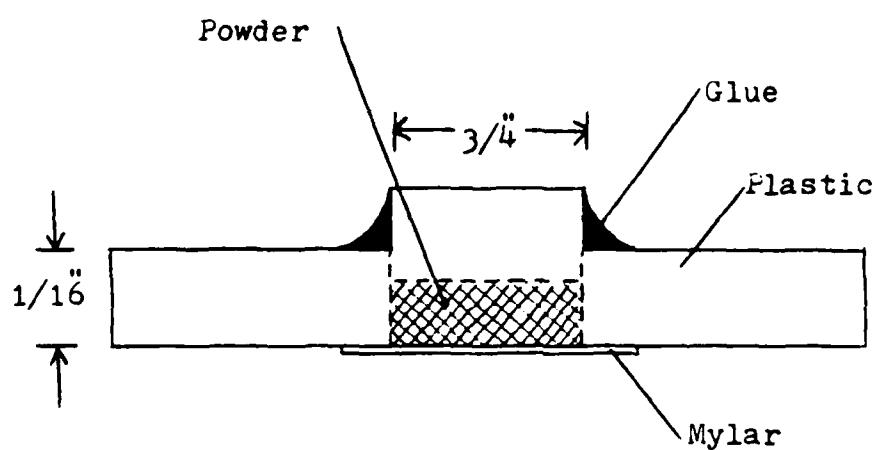
Figure 7. Powder Sample Preparation

a disk. The procedure for setting up and operating this system is included in appendix A.

## Absorber Parameters

The form of the alloy samples tested in this study include: 1) atomized powder, 2) cold compacted wafers, and 3) cold compacted-hot vacuum degassed wafers. All of the above absorber forms were fabricated to have the optimum grams per square centimeter as determined experimentally. By starting near the theoretically calculated optimum value, an improved value was found through succesive trial runs with powder absorbers of different $g/cm^2$. Each trial run was compared with the others by the relative intensity of the lines present. The range of values tested were between $0.05$ $g/cm^2$ and $0.15$ $g/cm^2$. From these tests, a value of $0.1$ $g/cm^2$ was chosen and applied to all other forms of the alloy samples.

The fabrication method of the powder test samples was chosen to provide a uniform density of powder across the area of the absorber. Of all the methods tried, only one was successful. This method consisted of putting a specific amount of powder into a 3/4 inch diameter hole which is in the center of a 1/16 inch thick , 2 inch square piece of plastic. One side of the hole was sealed with a piece of mylar bonded to the plastic with rubber cement. The other side was sealed with a 3/4 inch diameter 1/16 inch thick plastic disk resulting from the hole in the plastic sheet. This plug was lightly pressed into place with uniform pressure and the small space around the plug was then

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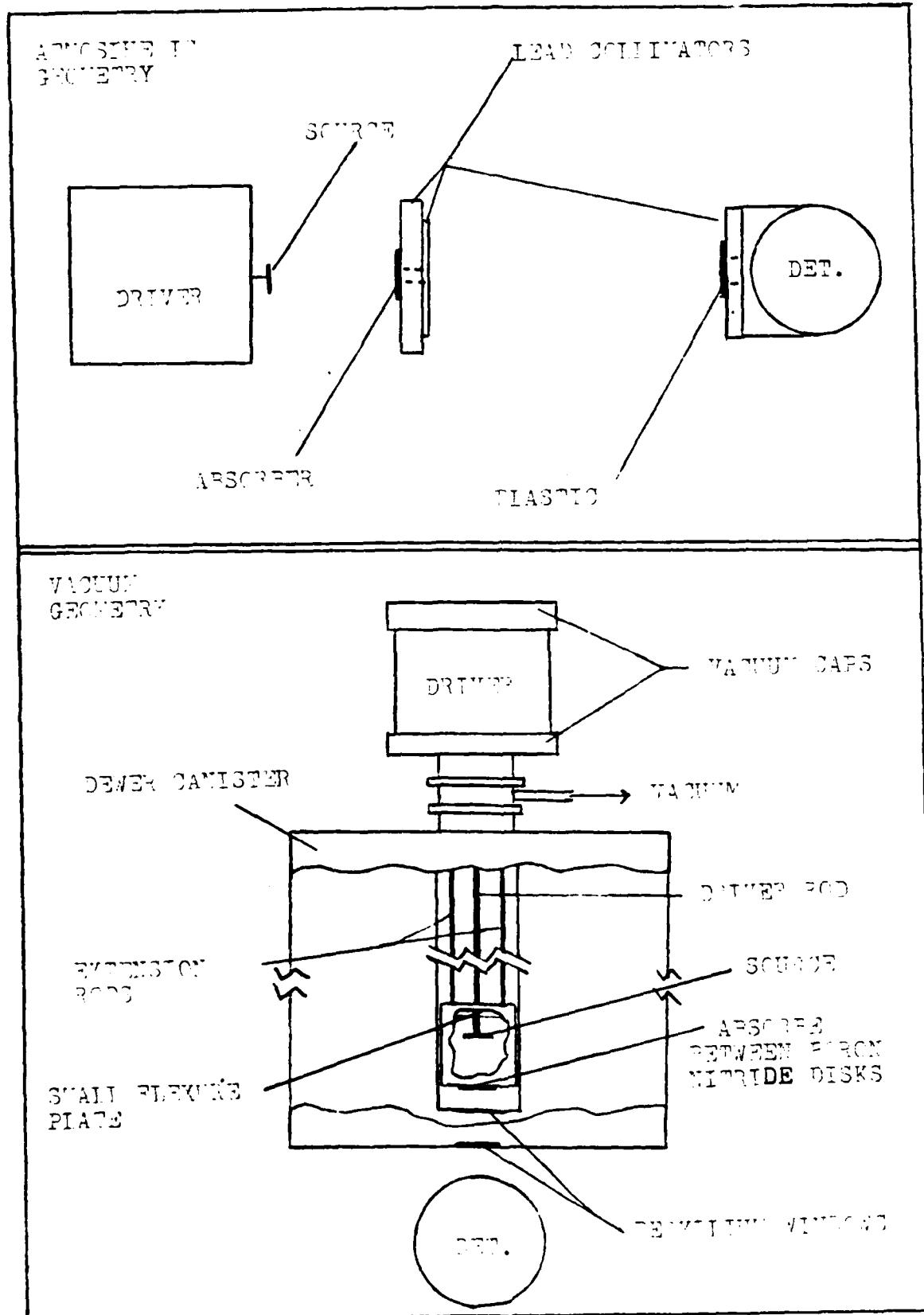
Figure 8. Experimental Geometry

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sealed with DUCO cement. with this method, the thickness in $g/cm^2$ was determined by dividing the weight of the powder inserted into the hole by the area of the hole.

The fabrication of the other samples was accomplished by the High Temperature Materials Branch at the Air Force Materials Laboratory. The cold compacted absorber was made by first putting a known amount of powder into a 1/16 inch thick cardboard die with a 1/2 inch diameter hole. The die and powder were then subjected to 24,000 pounds per square inch for approximately 15 seconds with a hydraulic hand press. The thickness in $g/cm^2$ was then determined by dividing the weight of the wafer by its area. By trial and error, a value of 0.102 $g/cm^2$ was obtained. The cold compacted-hot vacuum degassed samples were made by first repeating the above procedure to obtain a pressed wafer. These wafers were then placed in a vacuum chamber for two hours where a vacuum of 3E-05 Torr was reached. Next, still under vacuum, the samples were heated for 30 minutes at approximately 860 F. The samples were then cooled to 212 F in a period of about 1.5 hours with a final vacuum of 1.5E-05 Torr being reached. The samples were then removed from vacuum and were exposed to atmospheric conditions for 15 minutes before being placed in a vacuum dessicator at room temperature.

## Experimental Geometry

Due to component failure in the MS-900, all data for the alloy samples was obtained using the original Mossbauer system. The source used was 50 mCi cobalt-57 (date:5 June 1981)

diffused into a six micron thick rhodium matrix (8:8). The source was prepared by Amersham-Searle and produces, among other radiations, the 14.4 keV gamma ray of interest for this study. For the powder and cold compacted absorbers, the source-to-detector distance was 11.5 inches. A lead collimator with a 3/8 inch opening was placed 4 inches in front of the source, centered between the source and detector. The absorber was then placed on the front face of the collimator, centered over the hole. An additional lead collimator with a 7/8 inch opening was placed directly in front of the detector window and a plastic plate was placed over this hole to reduce the detection of 6.4keV X-rays emitted from the source.

For the cold compacted-hot vacuum degassed absorber, a vacuum system was used while aquiring data to insure that no properties of the hot vacuum degassing stage were changed by exposure to atmospheric conditions. The vacuum system was achieved by using a cylindrical dewar with a forepump and produced a vacuum of 2.79E-03 Torr. As can be seen in figure 8, the source to detector distance was reduced (to 6 inches) as well as the source to absorber distance (to 0.69 inches). Additionally, the plastic plate in front of the detector was removed because the new set-up has two berylium windows between the absorber and detector which is sufficient to absorb the 6.4 keV X-rays. For all three types of absorbers, the flyback mode was used and a run time of 48 hours was chosen to minimize statistical fluctuations in the spectra.

## IV.    Results and Discussion

In this section, the capabilities of the new computer based Mossbauer Spectrometer, as well as the results of all spectrum analysis will be presented. The spectra presented include calibration runs for both the new and original systems in addition to the spectra for each stage of alloy processing.

### System Capabilities

The capabilities of the new computer based Mossbauer spectrometer include simplified operation, a larger memory for data storage, and quicker data analysis. Unlike the original system, there is not an extensive network of cables connecting many separate system components, thus resulting in a simplified assembly. Also, in addition to a simplified assembly, the number of operating controls are reduced, so setting the system for operation is much easier and faster. Once the system is operating, the data can be manipulated with a joystick and by commands entered on the keyboard. Then, at any time during data acquisition, the APPLE 2+ can be used for normal functions totally independent of the MS-900. This is possible since the MS-900 has its own random access memory (RAM) of 1024 channels with 24 bits (16 million counts) each (11). Once all data needed is obtained, it can be stored on a 5 1/4 inch floppy disk, printed out, and/or sent to the PDP to be stored on an 8 inch floppy disk and analyzed. The time it takes to send the 1024 data points to the PDP is only 1 1/2 minutes whereas it took over an hour to manually type in the 400 point spectrum of the

original system. Once the data is available to the MOSFUN
program on the PDP, the same commands are used for analysis.
However, with 1024 data points instead of 400, all operations
take longer.

An example of a spectrum obtained by the new system and
analyzed by MOSFUN is shown in figure 2. This figure is that of
natural iron foil with respect to sodium nitroprusside. The
spectrum is shifted $0.243 \pm 0.006$ mm/s with respect to sodium
nitroprusside instead of the standard value of $0.26 \pm 0.002$ mm/s
(9). The calibration of this spectrum could be corrected by
acquiring data for natural iron foil for a longer period of time
than done previously and inserting the more accurate peak
channel locations into the DATI and DRIVE subroutines discussed
earlier. The current natural iron foil spectrum was obtained in
only 4.25 hours and thus the peak locations were subject to
statistical fluctuations. For a step by step guide for setting
up and operating the new system, see appendix A.

## Alloy Results

The results for the natural iron calibration run and
those for each stage of alloy proccessing are shown in table 3.
All isomer shifts in this table were adjusted to be relative to
natural iron. The spectra of the calibration run and those of
the alloy samples were obtained on the original Mossbauer
spectrometer as mentioned earlier, and are shown in figures
9-13. Thus, the velocity scale on all of these figures is
relative to cobalt 57 in a rhodium matrix.

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Table 3.

MOSFUN Results for Calibration and Alloy Samples With Respect to NFE

| Sample | Run Time (hrs) | Isomer Shift (mm/s) | Relative Peak Intensity (%) | Half Width (mm/s) | Peak Location (mm/s) |
|---|---|---|---|---|---|
| NFE Calibration (Original System) Peak # 1 | 21.9 | 0.000 | 26.2±4.7 | 0.144±0.011 | -5.280±0.037 |
| 2 | | | 21.9±5.2 | 0.140±0.012 | -3.056±0.027 |
| 3 | | | 13.2±10.6 | 0.132±0.020 | -0.832±0.025 |
| 4 | | | 13.2±10.6 | 0.132±0.020 | 00.832±0.023 |
| 5 | | | 21.9±5.2 | 0.140±0.012 | 3.056±0.018 |
| 6 | | | 26.2±4.7 | 0.144±0.011 | 5.280±0.024 |
| NFE Calibration (MJ-900 System) Peak # 1 | 4.25 | 0.000 | 15.99±3.3 | 0.180±0.009 | -5.316±0.026 |
| 2 | | | 14.68±4.0 | 0.149±0.009 | -3.077±0.018 |
| 3 | | | 8.32±7.5 | 0.144±0.016 | -0.344±0.013 |
| 4 | | | 8.32±7.5 | 0.144±0.016 | 0.344±0.017 |
| 5 | | | 14.68±4.0 | 0.149±0.009 | 3.077±0.013 |
| 6 | | | 15.99±3.3 | 0.180±0.009 | 5.316±0.013 |

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Table 3. (Continued)

| Sample | Run Time (hrs) | Isomer Shift (mm/s) | Relative Peak Intensity (%) | Half Width (mm/s) | Peak Location (mm/s) |
|---|---|---|---|---|---|
| Alloy Samples: | | | | | |
| Powdered Peak # 1 | 48 | $0.181\pm0.025$ | $19.78\pm3.2$ | $0.193\pm0.047$ | $-0.032\pm0.039$ |
| 2 | | | $20.90\pm3.3$ | $0.189\pm0.037$ | $0.395\pm0.069$ |
| Cold Compacted Peak # 1 | 48 | $0.181\pm0.031$ | $19.46\pm3.5$ | $0.193\pm0.064$ | $-0.029\pm0.04?$ |
| 2 | | | $21.10\pm3.7$ | $0.181\pm0.048$ | $0.390\pm0.041$ |
| Cold Compacted/ Hot Vacuum Degassed (Gaussian) Peak # 1 | 48 | $0.204\pm0.029$ | $17.88\pm2.5$ | $0.271\pm0.057$ | $-0.007\pm0.03$ |
| 2 | | | $20.36\pm3.9$ | $0.183\pm0.031$ | $0.416\pm0.067$ |
| Cold Compacted/ Hot Vacuum Degassed (Lorentzian) Peak # 1 | 48 | $0.206\pm0.078$ | $13.12\pm6.4$ | $0.173\pm0.029$ | $-0.109\pm0.050$ |
| 2 | | | $12.05\pm6.4$ | $0.173\pm0.029$ | $0.115\pm0.019$ |
| 3 | | | $19.91\pm2.4$ | $0.173\pm0.029$ | $0.411\pm0.058$ |
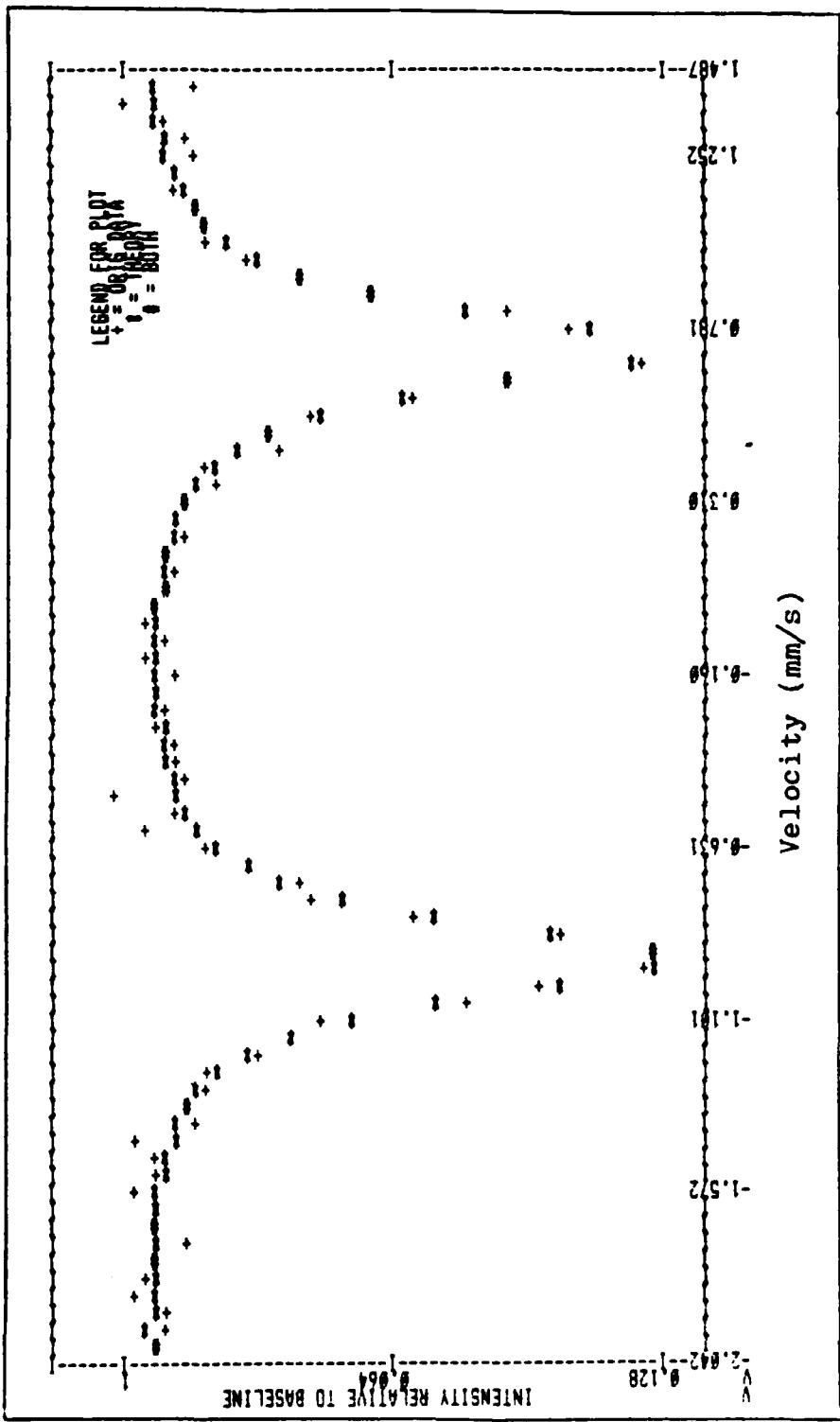
Figure 9. Natural Iron Results for Peaks 3 and 4 from Original Mossbauer Spectrometer (with respect to Co57 Source)
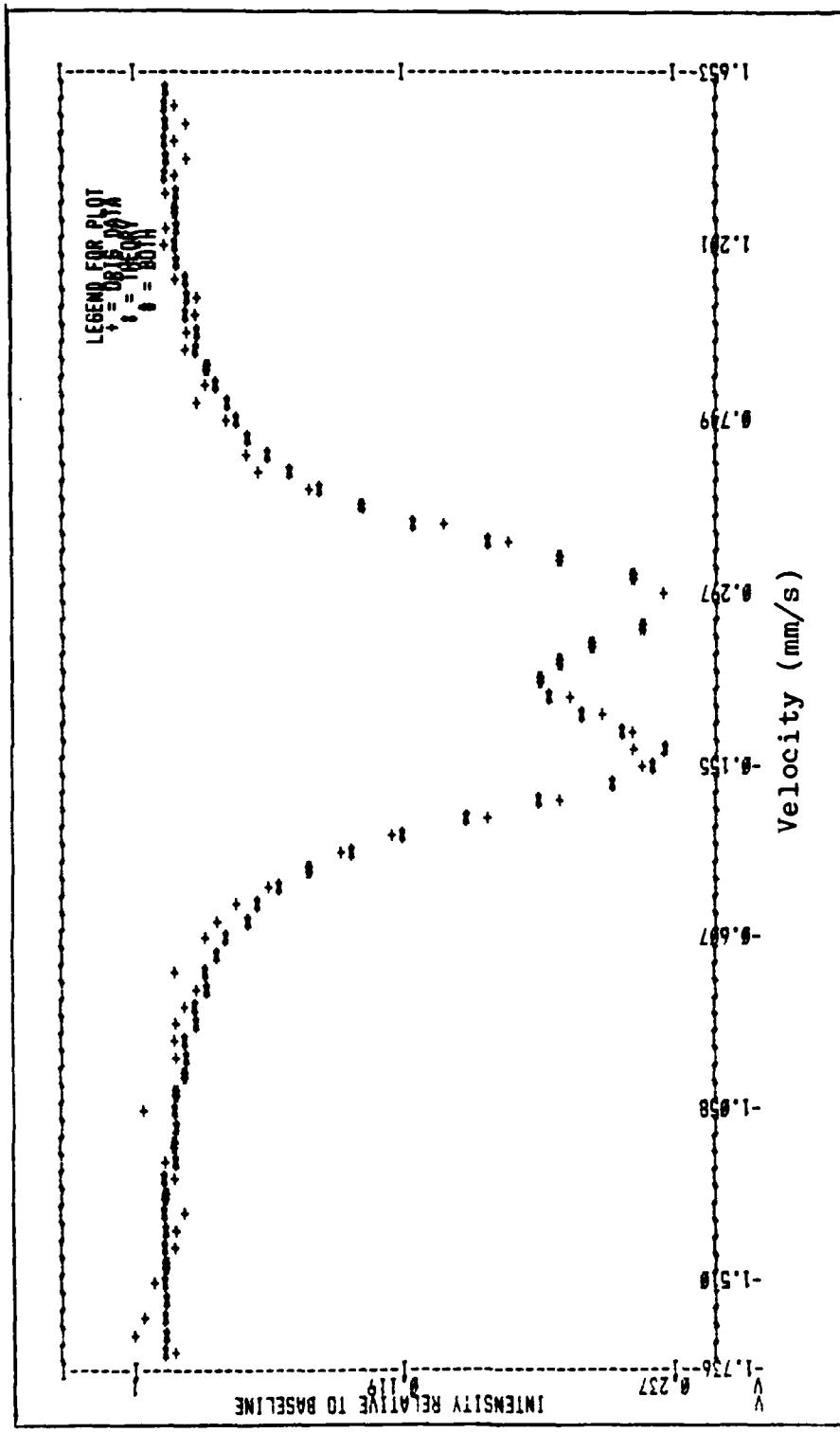
Figure 10. Results for Alloy Powder
(With respect to Co57 Source)

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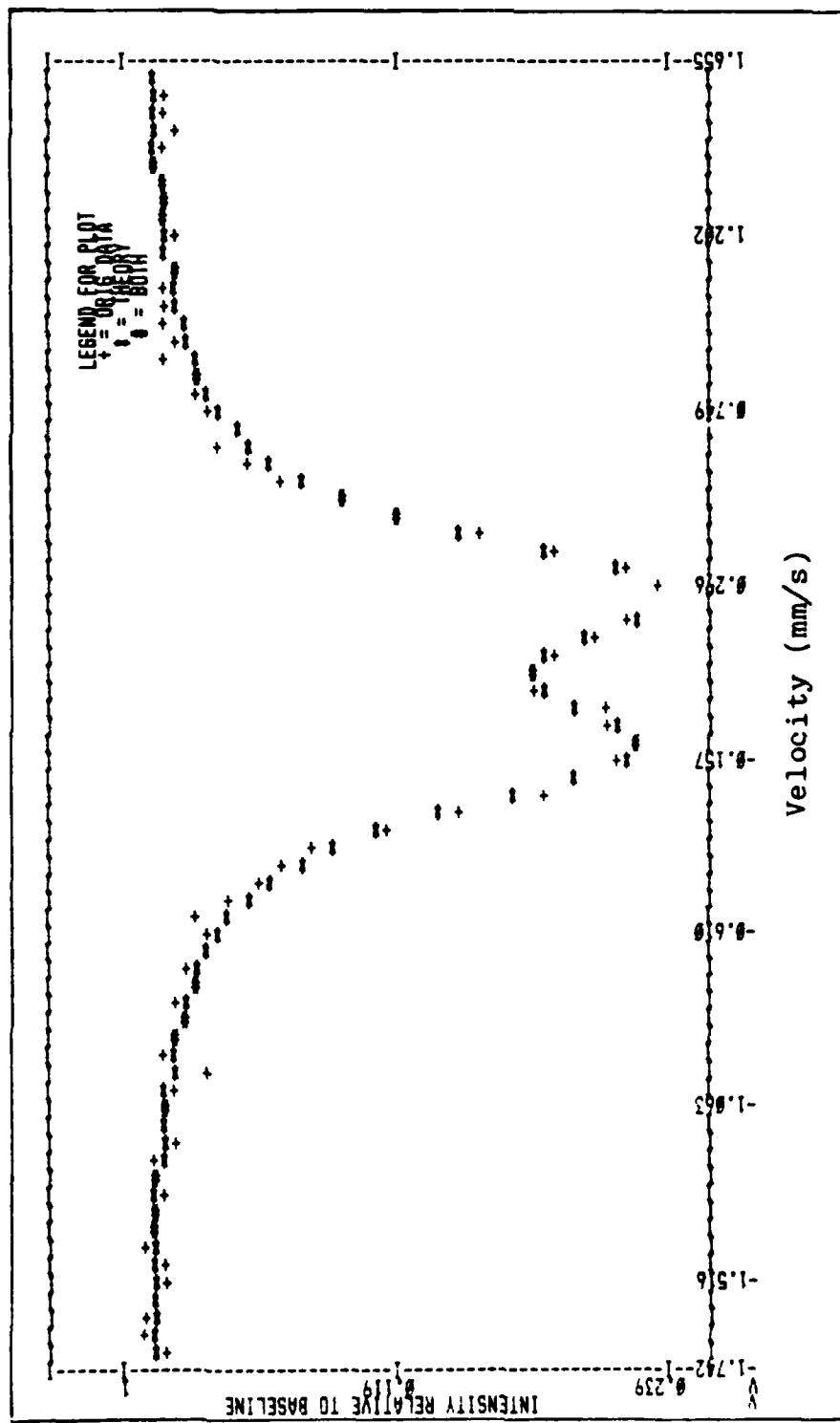
Figure 11. Results for Cold Compacted Alloy
(with respect to Co57 source)
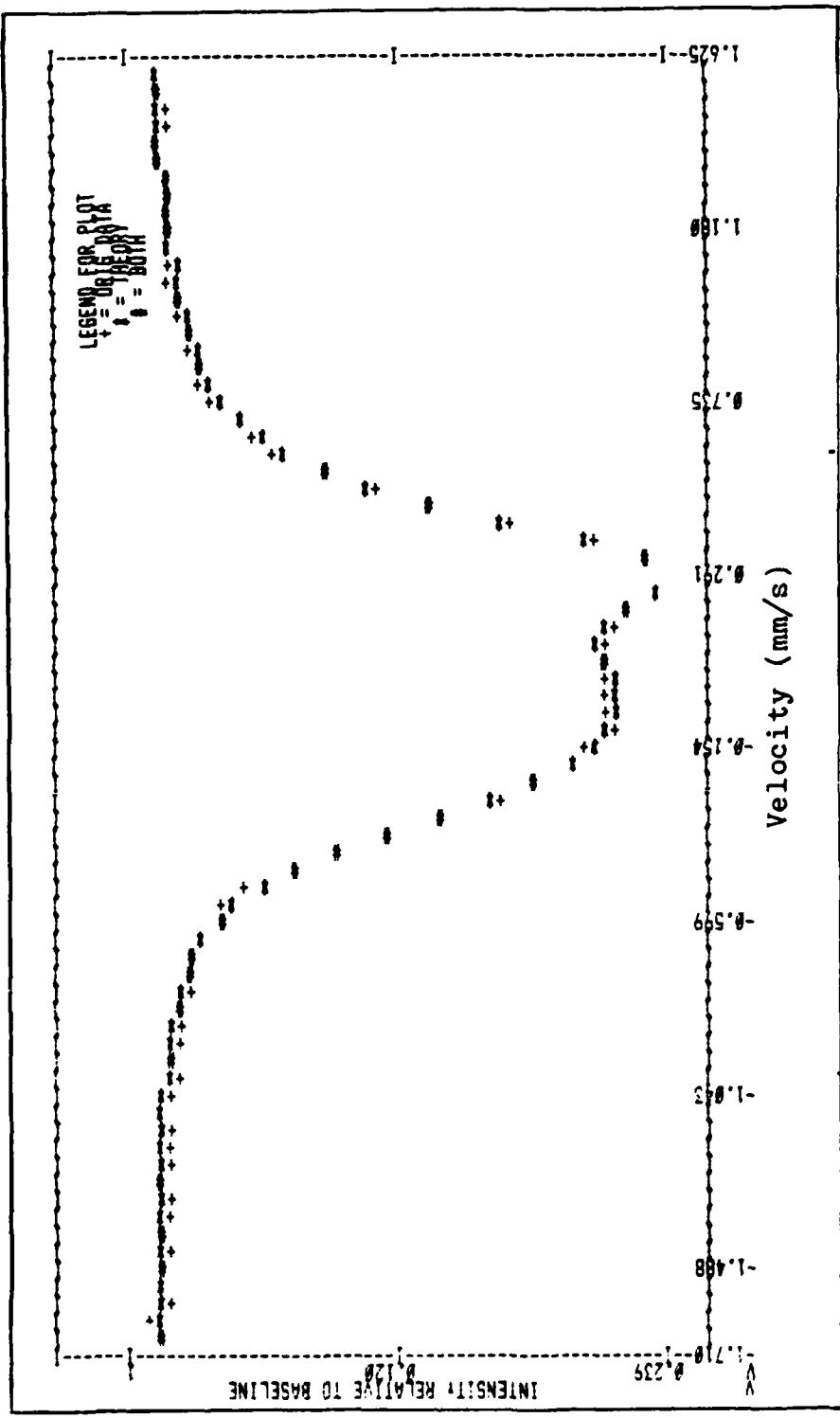
Figure 12. Results for Cold Compacted/Hot Vacuum Degassed Alloy (with respect to Co57 source)(2 line Gaussian fit)

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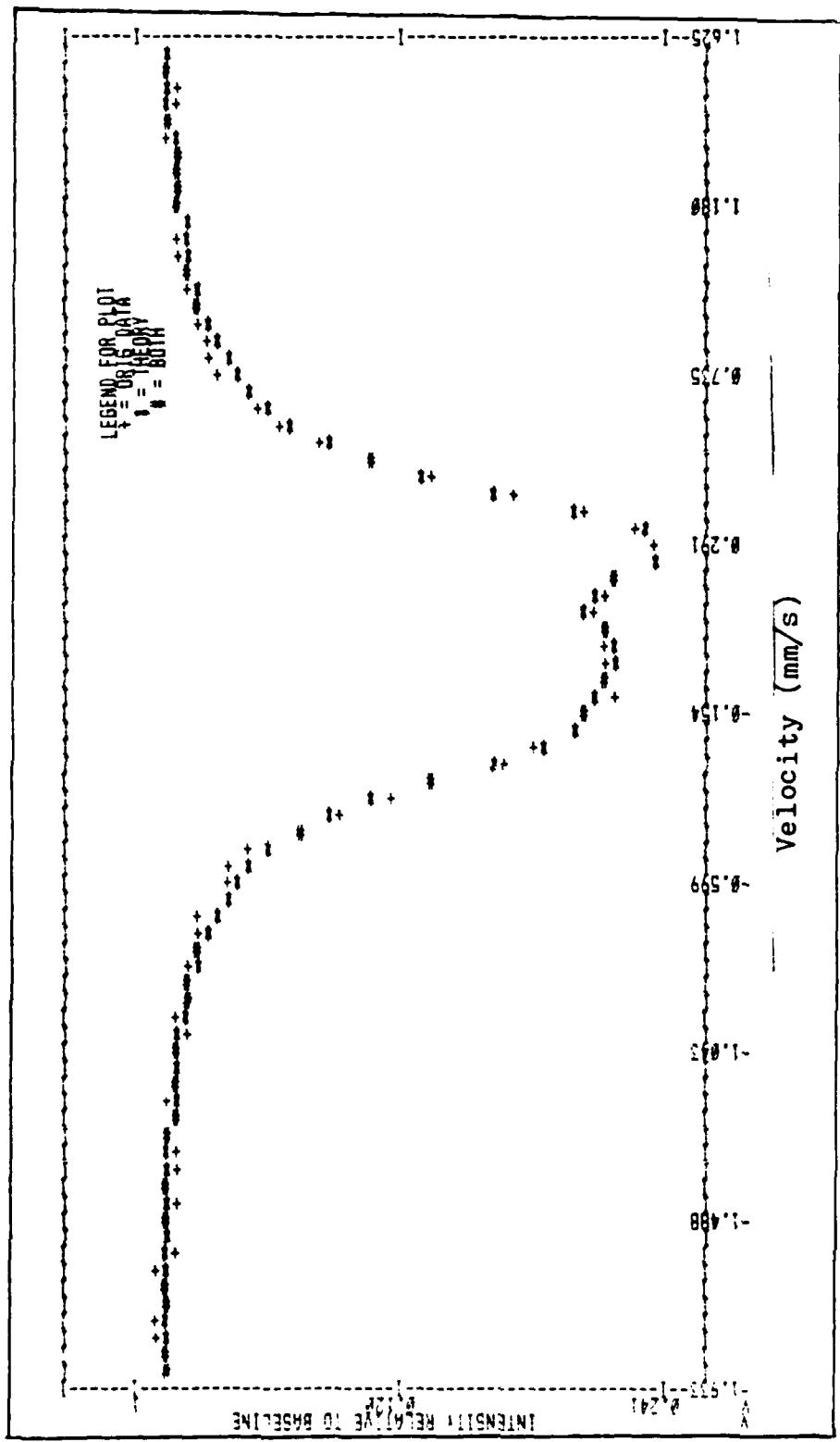
Figure 13. Results for Cold Compacted/Hot Vacuum
Degassed Alloy (with respect to Co57
source) (3 line Lorentzian fit)

All of the spectra shown here were fitted by MOSFUN using the Lorentzian-intensity theory with a gradient iteration refinement. The only exception was that of figure 12. This spectrum was fitted using the Voigt-Intensity theory for better results. The parameters varied to fit the spectra included: 1) baseline, 2) geometry factor (a measure of the amount of baseline curvature), 3) line intensity (each line independent of the other), 4) isomer shift, 5) quadrupole splitting (separation of doublet lines), and 6) half width at half maximum. In addition to these, an additional parameter, form, was assigned to each line of the Voigt fitted spectrum.

Figure 10 shows the spectrum of the atomized powder form of the alloy. As can be seen, the spectrum is that of a nearly symetric doublet. From this spectrum, it is not clear as to whether the doublet is a result of quadrupole splitting or two different compounds formed in the lattice. However, it is obvious that there is no hyperfine splitting present which indicates that agglomeration of iron atoms is unlikely. The cold compacted alloy results are shown in figure 11. Basically, the spectrum is identical to the powder alloy spectrum except for a slight decrease in the left peak intensity. However, due to the statistical errors of the parameter values, the peak intensities overlap and thus nothing conclusive can yet be stated as to whether quadrupole splitting is the mechanism present or whether a decrease in one of the two compounds occured. The results for the cold compacted-hot vacuum degassed samples are shown in figures 12 and 13. Due to the broadening of the left line, a new

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theory was needed to obtain a good fit. From figure 12 and table 3, it can be seen that the left peak has reduced in intensity and become more Gaussian shaped as opposed to Lorentzian. Even with statistical errors involved, the peak intensities are significantly different. In order to determine the cause of the left peak broadening and decrease in intensity, a new theory was considered. A spectra fit was attempted using three lines, letting each line's intensity and position vary independently. The results, shown in figure 13 and Table 3, indicate that the spectra is that of a quadrupole doublet (left two peaks) and a single line (right peak). Thus the left peak broadening is most probably due to quadrupole splitting. These results indicate that the two compound theory is the mechanism present. If this is the case, then only the third processing stage, which involved hot vacuum degassing, significantly changed the lattice structure. Although it is believed that two different compounds are present in the alloy, it is still not known what they are. The Fe $Al_6$ compound, which was expected to be seen, was not. Unfortunately, all efforts to match the peaks of this spectra to previous work on Al-Fe-Ce compounds has been unsuccesful.

## V.   Conclusions and Recomendations

### Conclusions

With the new system completed, Mossbauer spectra can
easily be obtained, displayed, and analyzed. In addition, the
system eliminates time normally wasted transferring data
manually. The only problems observed, other than the system
breaking down, were minor. These include poorly made front panel
switches and rear panel sockets, slow response from joystick
commands, and an incomplete instruction manual.

The spectra of the alloy samples show that two
compounds are formed in the gas atomization stage and remain
unchanged until the hot vacuum degassing stage. No spectra were
obtained for further processing stages due to a lack of prepared
samples. However, it is clear that Mossbauer spectrometry is
useful for following changes in the lattice structure due to
mechanical processing.

### Recommendations

There are several changes or additions possible which
would make the new system more valuable of a tool. First of all,
the MS-900 and VT-900 (motor) should be equipped with a Moire
interferometer to produce velocity data as the old system does.
If this is done, Pate's modified version of MOSFUN could be used
with minor changes. Secondly, the problems mentioned above
concerning faulty switches and sockets should be resolved by
replacing them. Thirdly, since the Physics Department of the Air
Force Institute of Technology has limited access to an APPLE 2+

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or 2e computer, it is recomended that the MS-900 be directly interfaced with the PDP 11/03. A brief discussion of the problems for this interfacing is included in appendix B. Fourth, it is recomended that the MOSFUN program be modified to accept triangular mode spectra.

As for the alloy studied, it is recomended that hot compacted-hot vacuum degassed and extruded samples be studied to follow the changes in the spectra due to these processing stages. Lastly, it is recomended that all samples be run at liquid nitrogen temperatures. This may result in new lines being revealed or sharpening of the present lines.

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APPENDIX A

## Assembly and Operating Instructons

### Assembly

1.  It is assumed that an APPLE 2+ Or 2e computer with a monitor
    is set up with a disk drive in slot #6, a printer (optional)
    in slot #1, and a joystick connected according to its
    specific instructions. Slots #2 and #4 should be vacant.

2.  Remove the top of the computer and place the Mossbauer
    interface card, MS-900-100, into slot #4 and bring the
    ribbon cable through the rear panel of the computer.

3.  Place the Super Serial Card, with the switch settings set as
    discussed earlier, into slot #2 of the computer and mount
    the female DB-25 connector into the rear panel of the
    computer.

4.  Place the cover back on the computer and connect the
    computer's power cord into the  upper  115 VAC OUT power
    outlet on the rear panel of the MS-900. Plug the monitor's
    power cord into the  lower  115 VAC OUT outlet.

5.  Making sure that the power on the MS-900 is OFF, connect the
    ribbon cable from computer slot #4 to the rear panel
    connector of the MS-900 labeled COMPUTER.

6.  Connect a mini-coax cable from the rear panel of the MS-900,
    marked 24V, to the connector marked POWER on the
    preamplifier.

7.  Connect a second mini-coax cable from the rear panel of the

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MS-900, marked ANALOG IN, to the connector marked OUTPUT on the preamplifier.

8. Connect a high voltage supply (not from MS-900) to the preamplifier/detector assembly.

9. Make sure that the three toggle switces marked EXT/INT are in the DOWN internal position and then connect the Mossbauer drive cable with the BLUE hexagonal connectors to the rear panel mating connector of the MS-900, labeled VT-900, and to the VT-900.

10. Connect the power cord to the female receptacle marked 115 VAC and plug the other end into the wall (power source).

11. Finally, connect one end of the 10 wire flat ribbon to the DB-25 connector of the Super Serial Card.

12. Refer to figure 14 for a block diagram of the system set-up.

Operation

1. With the power switch for the APPLE and monitor in the ON position, turn on the power switch on the front panel of the MS-900. The MS-900 controls the power system now.

2. Press the start button and the YELLOW light should come on.

3. Load the Mossbauer Master program into the disk drive and boot the program by typing PR#6 on the keyboard. The program menu should appear on the monitor.

4. Set the sampling time (time that a channel is open to receive data) to the desired value. The first two digits give the sampling time in microseconds, and the third digit is the multiplier in exponents of 10. A value of 200

microseconds is currently used.

5.  The lower level and upper level discriminators of the SCA
    are set in a modified pulse height analysis mode. This mode
    is engaged by pressing the PHA button ONCE. With the LLD set
    at the lowest value and the ULD set at the highest value,
    press the GREEN button marked STORE. Now press the A key to
    start data acquisition. The CLEAR button may be used to
    erase the spectrum at any time. The scale of the spectra can
    be increased or decreased by moving the joystick up or down.
    Once a spectrum is seen, identify the 14.4keV peak and
    adjust the gain until this peak is centered on the screen.
    At this point one should see a pulse-height spectrum with
    three numbers on the bottom of the screen. From left to
    right, these numbers are the channel number, number of
    counts in that channel, and the full scale number of counts
    displayed. To select the 14.4keV peak only, move the
    vertical line cursor to the left edge of the peak and
    increase the LLD until no more counts are seen on the left
    side of the cursor. The cursor is controlled by moving the
    joystick left or right. Now move the cursor to the right
    edge of the peak and decrease the ULD until no more counts
    are seen on the right side of the cursor. To stop acquiring
    data, press the STORE button again and the light should go
    out. Now press CLEAR to erase the memory. If the PHA button
    is pressed again, the light will still be on and the normal
    PHA mode is engaged.

6.  To obtain a Mossbauer spectrum, first press the ESC button
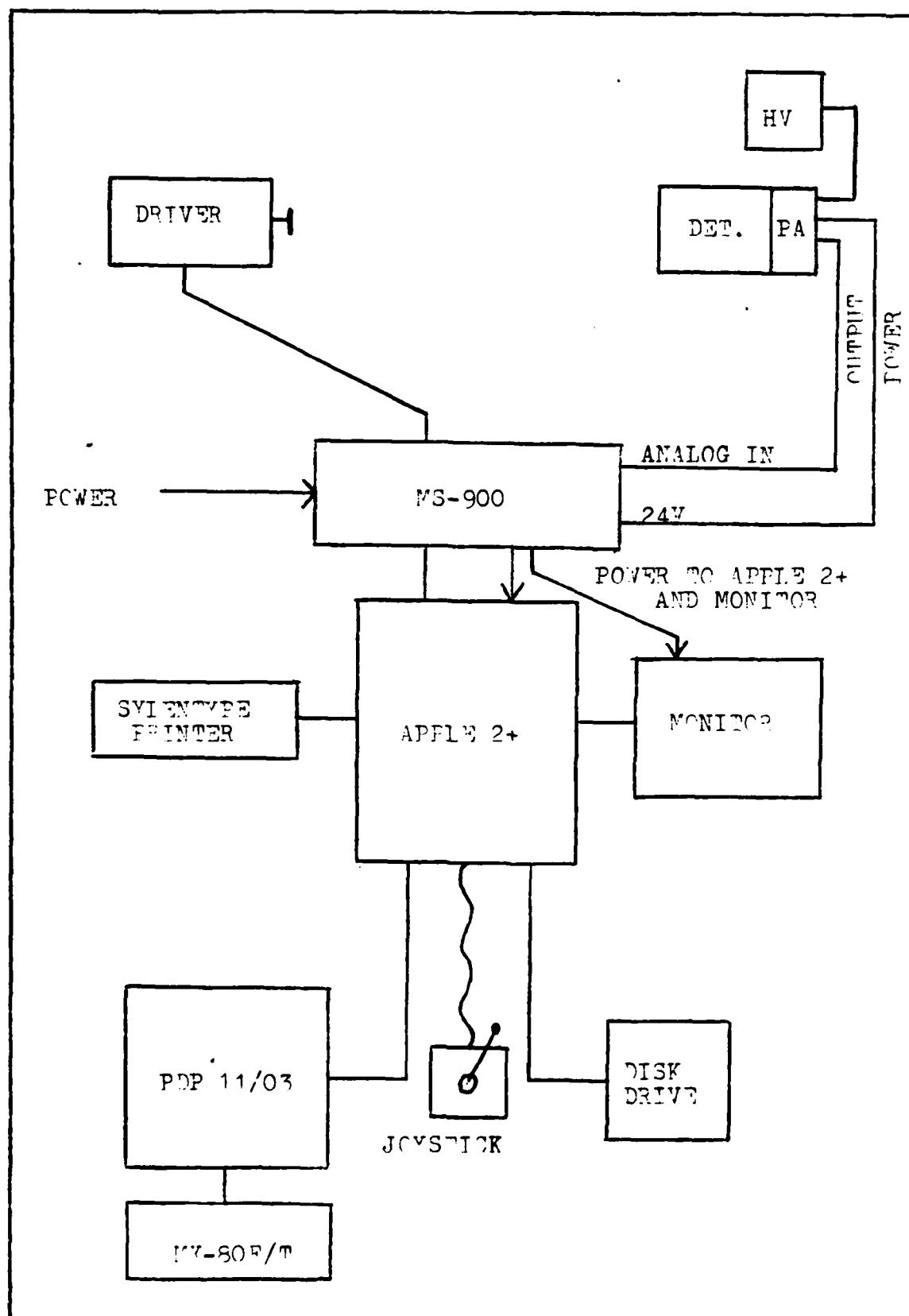
FIGURE 14. New Spectrometer Set-Up

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on the keyboard to return to the menu. Next, adjust the velocity values on the thumbwheel switches. For a full spectra, set the MAX VELOCITY to zero and the MIN VELOCITY to 6.0. Unlike the original spectrometer, these settings can be varied to produce a window though which only a part of the spectrum is acquired. Now press either the flyback or triangular mode button. The VT-900 driver should begin oscillating. The symmetry is now set by turning the symmetry potentiometer until the equilibrium position of the flexure plate is centered. Now, by pressing the STORE button and entering A on the keyboard, a Mossbauer spectrum should be seen.

7.  Other buttons on the front panel include SUB, SINGLE, TIME, and an unmarked blue button. The SUB button is used to subtract, instead of add, counts from the spectrum. With the STORE button OFF, a single subtraction scan can be executed by activating the SINGLE button and pressing the START button. The TIME button is activated to store the number of pulses from the crystal controlled clock. When not activated, the number of sweeps are recorded. In either case, this data is stored in the first two channels. The blue button is pressed to activate the acquiring of velocity data if a Moire interferometer is installed.

8.  At any time during operation, one can return to the menu by pressing the ESC key. This will not affect data acquisition at all. To use the APPLE for other purposes while data is being collected, return to the menu and type D for

displaying data. Then use CTRL-C to stop the program.
Finally, type TEXT to exit from the graphics mode.

9.  Once all data needed is acquired, simply deactivate the
    STORE button. Next, return to the menu and follow the
    diections given. To send the data to the PDP, choose the
    "print spectral data option". Before entering all the
    information requested by the program, boot the PDP and type
    EDIT FILENAME.EXT/C on the PDP terminal. Then disconnect the
    DB-25 connector from the back of the VT-100 and connect it
    to the male DB-25 at the other end of the 10 wire ribbon
    coming from the Super Serial Card. Now enter all information
    about the spectrum as prompted by the program. One should
    then have to wait 90 seconds until all data is transferred.
    Now one should reconnect the VT-100 to the PDP and save the
    file by using the GOLD 7-EXIT command of the keyboard
    editor.

10. Before the file can be analyzed, one defect in the file
    must be eliminated. When the data is sent over, an extra
    line is placed at the beginning of the file. This line must
    be deleted before the file can be analyzed.

11. If the data is that of a calibration spectra, the peak
    channel locations (a total of 6) should be entered into the
    DATI and DRIVE subroutines of MOSFUN. The peak locations can
    be found by printing the data file and manually searching
    for them. Once found, follow the directions at the beginning
    of the MOSFUN program for editing MOSFUN subroutines. A more
    detailed description is provided in appendix A of Pate's

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thesis.

12. Finally, to obtain a printout of the spectrum, the printer
    connected to the Apple should be used. The spectra printed
    by the MOSFUN program is very spread out since 1024 data
    points are plotted instead of 400. The ZOOM GRAPHICS program
    donated for use with an APPLE computer system is capable of
    printing spectra or parts of spectra in many different sizes
    and formats.

## Interfacing the MS-900 Directly to the PDP 11/03

An interfacing of the MS-900 directly to the PDP would result in a simplified operation and eliminate the need for an APPLE computer system. Once completed, the PDP would perform all of the functions previously done by the APPLE and there would not be a need to connect/disconnect cables in order to send data to the PDP.

The work involved for this interfacing involves both hardware connections and software changes. From discussions with Captain Paul Bailar, U.S.A.F, who had previously worked on a spectrometer - computer interfacing, a basic outline of the problem was obtained (12). First, the interface card for the MS-900 should be studied to understand exactly what functions it performs. This would enable one to build a similar interface for joining the MS-900 and the PDP. Second, once a hardware connection is made, software will have to be written for the PDP so that it may understand the signals sent from the MS-900. Third, the Mossbauer Master program will have to be studied so that it may be re-written for the PDP. The current version is written in BASIC for an APPLE computer and uses machine specific commands. Thus, a simple translation to FORTRAN is not possible. Finally, in order for the spectra to be displayed on a terminal as it is currently done, graphics capability will have to be added to the VT-100 or the VT-100 can be replaced with a VT-55

terminal. In either case, the FORTRAN version of the Mossbauer

Master program should permit the joystick functions to be

replaced by keyboard commands.

APPENDIX C

Listings For:

Mossbauer Master program

Subroutine DATI

Subroutine DRIVE

```
2   HIMEM: 34300
6   TEXT
7   POKE 961,0: POKE 962,0: POKE 975,5
10  D$ =  CHR$ (13) +  CHR$ (4)
20   TEXT : HOME
30   PRINT "           MS-900": PRINT
40   PRINT "MOSSBAUER SYSTEM"
50   PRINT : PRINT : PRINT
60   PRINT "(A)QUIRE SPECTRAL DATA": PRINT
70   PRINT "(S)TORE  SPECTRAL DATA ON DISK": PRINT
80   PRINT "(R)ETRIEVE SPECTRAL DATA FROM DISK": PRINT
90   PRINT "(P)RINT SPECTRAL DATA": PRINT
100   PRINT "(T)RANSMIT SPECTRAL DATA": PRINT
105   PRINT "(D)ISPLAY SPECTRAL DATA": PRINT : PRINT
110   PRINT : PRINT "PLEASE SELECT ONE OF THE ABOVE"
120   PRINT : GET A$
125   HOME
130   IF A$ = "A" THEN 1010
140   IF A$.= "R" THEN 3000
150   IF A$ = "S" THEN 2008
160   IF A$ = "D" THEN 4000
170   IF A$ = "P" THEN 4500
250   GOTO 20
1010   IF  PEEK (34688) = 8 THEN  GOTO 2004
1030   GOTO 2003
1900   PRINT "1111111111111111111111111111111111111111111111111111111111111111111111
       11111111111111111111111111111111111111111111111111111111111111111111111111111
       11111111111111111111111111111111111111111111111111111111111111"
2000   PRINT "2222222222222222222222222222222222222222222222222222222222222222222222
       2222222222222222222222222222222222222222222222222222222222222222222"
2001   PRINT "3333333333333333333333333333333333333333333333333333333333333333333333
       33333333333333333333333333333333333333333333333333333333333333333333333333333
       3333333333333333333333333333333333333333333333333333333333333"
2003   PRINT D$;"BLOAD HISPDDATAGRAB"
2004   CALL 34688
2005   GOSUB 5000
2006   GOTO 2004
2008   PRINT "WHAT IS THE NAME OF THE DATA"
2010   PRINT "TO BE SAVED ON THE DISK ?": PRINT : PRINT
2020   INPUT " ";A$
2030   PRINT : PRINT : PRINT : PRINT "DATA GOING OUT TO DISK"
2040   PRINT D$;"BSAVE ";A$;",A$8900,L$C00"
2050   GOTO 20
3000   PRINT "WHAT IS THE NAME OF THE DATA"
3005  D$ =  CHR$ (4)
3010   PRINT "TO BE RETRIEVED FROM              THE DISK ?": PRINT
       : PRINT
3020   INPUT " ";A$
3025   PRINT : PRINT : PRINT : PRINT "DATA COMING IN FROM DISK"
3030   PRINT D$;"BLOAD ";A$
3050   GOSUB 5000
3060   GOTO 3050
4000   GOSUB 5000
4010   GOTO 4000
4500   TEXT : PRINT "WHAT IS THE NAME OF THE SPECTRUM ?"
4510   INPUT " ";A$
```

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```
4511    INPUT "ENTER TOVR,NOVR,N,PERI,NDRV SEPARATED BY COMAS.";TV,NO,N,PE,N
        D
4512    INPUT "FORMAT? (EX. 8F9.0) ";F$
4520    INPUT "SEND DATA TO SILENTYPE OR PDP-11? (1 OR 2):";Z
4521    PR# Z
4530    PRINT : PRINT A$
4531    PRINT F$
4532    PRINT TV;",";NO;",";N;",";PE;",";ND;",";MP;",";NS
4540 BASE = 35072
4550    FOR T = 0 TO 3048 STEP 24
4570    FOR S = 0 TO 21 STEP 3
4580 X =  PEEK (BASE + T + S) +  PEEK (BASE + T + S + 1) * 256 +  PEEK (BA
        SE + T + S + 2) * 65536
4581    IF X < 10000000 THEN Q = 3
4582    IF X < 1000000 THEN Q = 4
4583    IF X < 100000 THEN Q = 5
4585    IF X < 10000 THEN Q = 6
4586    IF X < 1000 THEN Q = 7
4587    PRINT  SPC( Q - 1)X;
4590    NEXT S
4600    PRINT
4605    IF  PEEK (49152) = 155 THEN 4620
4607 Q = 0
4610    NEXT T
4620    PR# 0
4630    GOTO 20
5000    REM  DISPLAY SUBROUTINE
5005    IF  PEEK (2783) <  > 160 THEN  GOSUB 6000
5010    IF  PEEK (34304) = 162 THEN 5030
5020    PRINT : PRINT D$;"BLOAD JOYSTICK"
5030    CALL 34304
5040 BASE = 35072
5042 CH =  PEEK (961) +  PEEK (962) * 256
5045 C3 = CH * 3
5050 COUNT =  PEEK (C3 + BASE) +  PEEK (C3 + BASE + 1) * 256 +  PEEK (C3 +
        2 + BASE) * 65536
5055    VTAB (21)
5057    PRINT "                    ";: HTAB (27): PRINT "          ";
5058    HTAB (1)
5060    PRINT CH;: HTAB (10): PRINT COUNT;: HTAB (24): PRINT 2 ^ (24 -  PEEK
        (975));"  FS"
5070    FOR T = 0 TO 39
5080    POKE 2640 + T, PEEK (1616 + T)
5090    NEXT
5100 A =  PEEK (49152)
5110    IF A <  > 155 THEN  RETURN
5120    GOTO 20
6000 T = 2640:U = 2768:V = 2896:W = 3024
6010    FOR S = 0 TO 39
6020    POKE (S + T),160
6030    POKE (S + U),160
6040    POKE (S + V),160
6050    POKE (S + W),160
6060    NEXT S
6070    RETURN
```

```fortran
        SUBROUTINE DATI (N1,N2,N3)
C
        COMMON /UNIT/ NRD,NWR,NCR,LFR,LFD,NFL,NVS,MAXN,MAXM,MAXF,NV(121)
        COMMON /DAT/  VMAX,PERI,Y(1024),ID(40),NDRV,N,NF,VEL(10)
        COMMON /THEO/ F,P(32),DF(32),NTEO,M,MF,KTEO(20),KP(32)
        COMMON /FLD/  P3,B,V,VCON(65),V1,V2,GEO,B0,C0,NFLD,MSH,MPLEX,1(HI
        COMMON /TRA/  IN(81),OUT(16)
C
        DIMENSION KFRM(8),IFRM(8),INST(4)
        DATA IFRM/2H(1,2H0F,2H8.,2H0),2H  ,2H  ,2H  ,2H  /
        DATA INST(1)/1HL/,INST(2)/1HZ/,INST(3)/1HH/,INST(4)/1H*/
        DATA NY/1HY/
C
C       N1 = INPUT UNIT
C       N2 = FACTOR FOR SEARCHING DROPPED CHANNELS
C       N3.NE.0 ERROR RETURN
C
        N9=N2
        IF(N1.EQ.0) GOTO 285
        READ(N1,5200,END=202)(ID(I),I=1,40)
        READ(N1,5200,END=202)(KFRM(I),I=1,8)
        READ(N1,5210,END=202)(IN(I),I=1,80)
        GOTO 203
C
C       EOF
C
  202   WRITE(NWR,6205) N1
        N=0
        N3=1
        RETURN
  203   CALL TRANS(NN)
        IOVR=OUT(1)
        NOVF=OUT(2)
        N=OUT(3)
        PERI=OUT(4)
        NDRV=OUT(5)
C       MPLEX=OUT(6)
C       NST=OUT(7)
        NST=189
  285   IF (N.EQ.0) N=1024
C
C       MORE THAN MAXN POINTS
C
        IF(N.LE.MAXN) GOTO 220
        N=0
        N3=1
        WRITE(NWR,6200) MAXN
        RETURN
  220   IF(NDRV.EQ.0) NDRV=3
        IF(PERI.EQ.0.) PERI=N*2.
C       IF(NST.EQ.0) NST=189
        P3=PERI * .5 + .5
  230   IF(IFRM(1).NE.IFRM(8)) GOTO 240
        DO 231 I=1,8
  231   IFRM(I)=IFRM(I)
```

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```
   240     WRITE(NWR,6230) (ID(I),I=1,39)
           WRITE(NWR,6240) TOVR,NOVF,N,PERI,NDRV,KFRM
           DO 241 I=1,MAXN
   241     Y(I)=0.
           READ(N1,KFRM,END=250) (Y(I),I=1,N)
C

C          CALCULATE AVERAGE TIME OSC. COUNTS
C
    99     TIME=0.
           DO 100 I=1,2
           TIME=TIME+Y(I)+16777216.*TOVR
   100     Y(I)=0.
           TIME=TIME/2
C
C          Fe57 peaks 1 thru 6 (mm/sec) w/respect to SNP.
           VCON(2)=-5.0494
           VCON(3)=-2.8167
           VCON(4)=-0.5800
           VCON(5)=1.1007
           VCON(6)=3.3376
           VCON(7)=5.5754
C
C          Y(I) where I=channel numbers for above peaks. From NFECAL.EXT
C          18-NOV-83 on MS-900.
           Y(189)=0.
           Y(331)=0.
           Y(476)=0.
           Y(582)=0.
           Y(733)=0.
           Y(878)=0.
C
C          Use GOTO statement to by-pass normal velocity extraction from
C          data.
           GOTO 107
C
C          EXTRACT VELOCITY DATA, ACCOUNT FOR
C          OVERFLOWS AND ZERO AFTER PUTTING IN VCON.
C
           IIII=0
           III=0
           NEND=PERI/2
           DO 101 I=19,NEND,MPLEX
           VJMP=Y(I+MPLEX)-Y(I)
           IF(VJMP.GE.500000.) III=III+1
   101     CONTINUE
           J=1
           DO 102 I=NST,NEND,MPLEX
           J=J+1
           IF(III.EQ.0) GOTO 105
           VJMP=Y(I+MPLEX)-Y(I)
           IF(J.GT.65) GOTO 102
           VCON(J)=Y(I)+FLOAT(III)*16777216.
           IF (VJMP.GE.500000.) III=III-1
```

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```
           GOTO 102
  105      VJMP=Y(I)-Y(I+MPLEX)
           IF(J.GT.65) GOTO 102
           VCON(J)=Y(I)+FLOAT(IIII)*16777216.
           IF(VJMP.GE.500000.) IIII=IIII+1
  102      Y(I)=0.
           Y(399)=0.
           III=-1
           DO 106 I=3,J-1
           VJMP=ABS(VCON(I-1))-VCON(I)
           IF(ABS(VCON(I)-VCON(I+1)).GT.(2.*VJMP)) III=1
           VCON(I)=VCON(I)*FLOAT(III)
  106      CONTINUE
           VCON(2)=-VCON(2)




  107      VCON(1)=7
           NN=N1
           NK=N2
           N1=0
           N2=NST
           CALL DRIVE(N1,N2)
           N1=NN
           N2=NK
           GOTO 260
C
C          LESS THAN N DATA IN PARTITION N1
C
  250      WRITE(NWR,6210) I,N
           DO 255 J=I,N
  255      Y(J)=0.
           GOTO 99
C
C          ADD OVERFLOWS, ZERO CHANNELS OUT OF RANGE
C
  260      IF(N1.NE.NCR) REWIND N1
           MSH=0
           G4=16777216.*FLOAT(NOVF)
           IF(NOVF.LT.0) G4=-1048576.*FLOAT(NOVF)
           IF(N9.EQ.0) GOTO 264
           DO 262 I=3,N
           IF(Y(I).NE.0.) GOTO 263
  262      CONTINUE
  263      G2=N9
           G3=Y(I)+G4
           G2=SQRT(G3+G4)*G2
  264      DO 280 I=1,N
           IF(Y(I).EQ.0.) GOTO 280
           Y(I)=Y(I)+G4
           IF(N9.EQ.0) GOTO 280
           IF(ABS(Y(I)-G3).LE.G2) GOTO 275
```

```
              WRITE(NWR,6220) I,Y(I)
              IF(NVS.EQ.0) GOTO 270
      265     WRITE(NWR,9000)
              READ(NRD,5210,END=265)JJ
              IF(JJ.NE.NY) GOTO 280
      270     Y(I)=0.
              GOTO 280
      275     G3=Y(I)
      280     CONTINUE
C
C             ZERO CHANNELS, FIT INTERVALS, GENERATE HALF SPECTRA
C
      285     DO 286 I=1,N
      286     Y(I)=ABS(Y(I))
      290     IF(NVS.EQ.0) GOTO 287
              WRITE(NWR,9210)
              NN=PERI
              IF(N.LT.NN) GOTO 287
              WRITE(NWR,9215)
      287     READ(NRD,5210,END=290) NN
              DO 291 K=1,4
              IF(NN.EQ.INST(K)) GOTO 294
      291     CONTINUE
C
C             INVALID INPUT
C
              IF(NVS.EQ.1) GOTO 290
      292     WRITE(NWR,6275)
              N3=1
              RETURN
      294     GOTO (295,295,320,340),K
      295     IF(NVS.EQ.1) WRITE(NWR,9220)
              READ(NRD,5210,END=295) (IN(J),J=1,NPL)
              IF(IN(1).EQ.INST(4)) GOTO 290
              CALL TRANS(NN)
              IF(NN.EQ.0) GOTO 290
              K1=ABS(OUT(1))
              K2=ABS(OUT(2))
              IF(K2-K1) 300,302,302
      300     NN=K1
              K1=K2
              K2=NN
      302     IF(K2.GT.N) GOTO 295
              IF(K1.EQ.0) K1=K2
              IF(K1.EQ.0) GOTO 295
              KK=K-2
              IF(KK.EQ.-1) WRITE(NWR,6250) K1,K2
              IF(KK.EQ.0)  WRITE(NWR,6260) K1,K2
              DO 304 J=K1,K2
      304     Y(J)=FLOAT(KK)*ABS(Y(J))
              GOTO 295
      320     NN=PERI
              IF(N.LT.NN) GOTO 290
```

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```
              IF(NVS.EQ.1) WRITE(NWR,9240)
              KF(3)=0
              READ(NRD,5210) KK
              IF(KK.EQ.INST(1)) GOTO 330
              NN=N/2
              DO 325 I=1,NN
              G1=Y(I)
              II=N-I+1
              Y(I)=Y(II)
  325         Y(II)=G1
  330         N=N/2
              WRITE(NWR,6270) N
              GOTO 290
  340         NF=N
              DO 350 I=1,N
              IF(Y(I)) 345,345,346
  345         NF=NF-1
              GOTO 350
  346         B=Y(I)
  350         CONTINUE
              NFLD=0
              RETURN
C     ***********************************************************************
  5200        FORMAT(40A2)
  5210        FORMAT(80A1)
C     ***********************************************************************
  9000        FORMAT(1H0,'ZERO Y/N'/)
  9200        FORMAT(1H0,F5.0,' TIME OVERFLOWS',',',I5,' DATA OVERFLOWS'/)
  9210        FORMAT(1H0,'* = END'/' Z = ZERO CHANNELS'/' L = SET FIT LIMITS'/)
  9215        FORMAT(1H ,'H = GENERATE HALF PERIOD SPECTRUM'/)
  9220        FORMAT(1H ,'CHANNEL 1, CHANNEL 2'/)
  9240        FORMAT(1H ,'L = LEFT, R = RIGHT HALF'/)
C
  6200        FORMAT(1H0,'***** ERROR ***** MORE THAN',I5,' POINTS')




  6205        FORMAT(1H0,'***** ERROR ***** EOF ON UNIT',I3)
  6210        FORMAT(1H0,'**** WARNING **** POINTS',I5,' TO',I5,' ZEROED')
  6220        FORMAT(1H0,'**** WARNING **** POINT',I4,' OUT OF RANGE',F10.0)
  6225        FORMAT(1H0,'**** WARNING **** VELOCITY OVERFLOW PROBLEM')
  6230        FORMAT(1H0,1H ,39A2)
  6240        FORMAT(1H0,4X,'TIME OVERFLOWS',F6.0,/5X,'DATA
             1 OVERFLOWS',I5/5X,'CHANNELS',7X,I5/5X,
             2'PERIOD',7X,F10.3/5X,'DRIVE MODE',6X,I3/5X,
             3'INPUT FORMAT   ',8A2)
  6250        FORMAT(1H0,I4,' -',I4,' NOT FITTED')
  6260        FORMAT(1H ,I4,' -',I4,'ZEROED')
  6270        FORMAT(1H ,'HALF PERIOD SPECTRUM ',I5,' CHANNELS')
  6275        FORMAT(1H ,'***** ERROR ***** INVALID INPUT')
              END
```

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```
          SUBROUTINE DRIVE (N1,N2)
          COMMON /UNIT/ NRD,NWR,NCR,LPR,LFD,NFL,NVS,MAXN,MAXM,MAXF,NV(121)
          COMMON /DAT/  VMAX,PERI,Y(1024),ID(40),NDRV,N,NF,VEL(10)
          COMMON /THEO/ F,P(32),DF(32),NTEO,M,MF,KTEO(20),KF(32)
          COMMON /FLD/  P3,B,V,VCON(65),V1,V2,GEO,B0,C0,NFLD,MSH,MPLEX,TIME
          COMMON /TRA/  IN(81),OUT(16)
          COMMON /LIN/  BB(32),A(32,32)
C
          DIMENSION X(65),XY(65),XDP(10),XYDP(10)
C
C         N1 = 0   CALCULATE VELOCITY COEFF.
C         N1 = 1   VELOCITY V FROM CHANNEL NUMBER XX
C         N1 = 2   V,GEO
C         N1 = 3   DERIVATIVES P(1)-P(3)
C         N1 = 4   DERIVATIVES P(1)-P(2)
C
C         N2 = 1st CHANNEL CONTAINING VELOCITY  (N1=0)
C         N2 = CHANNEL NUMBER     (FOR N1 = 1-4)
C         N2 = 0   ERROR RETURN
C
C         NDRV = 1   TRIANGULAR WAVE MODE
C         NDRV = 2   SINE WAVE MODE
C         NDRV = 3   FLYBACK WAVE MODE**
C
          IF(N1.NE.0) GOTO 1000
          NST=N2
          NFN=VCON(1)
          GOTO (1,2,3), NDRV
    1     WRITE(NWR,6000)
          RETURN
    2     WRITE(NWR,6200)
          VCON(1)=0.
          RETURN
    3     WRITE(NWR,6300)

C         Channel numbers for NFECAL.EXT peaks 1 thru 6.

          X(2)=NST
          X(3)=331.0
          X(4)=476.0
          X(5)=582.0
          X(6)=733.0
          X(7)=878.0
C         XY(2)=VCON(2)*156.25/TIME
          XY(2)=VCON(2)
          DO 401 I=3,NFN
C         X(I)=X(I-1)+MPLEX
C401      XY(I)=VCON(I)*156.25/TIME
  401     XY(I)=VCON(I)
          L=2
          K=1
```

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```
C
C          FIND MIN AND MAX VALUES FOR X
C
           XMIN=X(2)
           XMAX=X(2)
           DO 402 I=3,NFN
           XMIN=AMIN1(XMIN,X(I))
  402      XMAX=AMAX1(XMAX,X(I))
C
C          ZERO ARRAYS FOR SUMMING
C
           MM=2*K+1
           DO 403 I=1,MM
           XDP(I)=0.
           XYDP(I)=0.
  403      CONTINUE
C
C          TRANSFORM RANGE OF X TO (-1,1) AND COMPUTE SUMS OF
C          POWERS OF X AND SUMS OF XY TIMES POWERS OF X.
C
           C1=2.0/(XMAX-XMIN)
           C2=(XMAX+XMIN)/(XMAX-XMIN)
           LU=2*K+1
           LL=K+2
           DO 404 II=2,NFN
           XP=1.
           XI=C1*X(II)-C2
           DO 405 I=1,L
           XDP(I)=XDP(I)+XP
           XYDP(I)=XYDP(I)+XP*XY(II)
  405      XP=XP*XI
           DO 404 I=LL,LU
           XDP(I)=XDP(I)+XP
  404      XP=XP*XI
           DO 406 I=1,L
           BB(I)=XYDP(I)
           DO 406 J=1,L
           A(I,J)=XDP(I+J-1)
  406      CONTINUE
C
C          CALL LINEQ AND FIT VELOCITY DATA
C
           N1=0
           N2=2
           CALL LINEQ(N1,N2)
C
C          MOVE VELOCITY CALIB. TO VEL ARRAY
C
           DO 407 I=1,L
           JK=K-I+2
  407      VEL(JK)=BB(I)
C
C          ADJUST COEFF. TO ORIGINAL RANGE OF X
C
```

```
          DO 408 I=1,K
          DO 408 J=1,I
  408     VEL(J)=VEL(J)*C1
          C1=(XMAX+XMIN)/2.0
          DO 409 I=1,K
          MM=L-I+1
          DO 409 J=2,MM
  409     VEL(J)=-C1*VEL(J-1)+VEL(J)
C
C         COMPUTE MAXIMUM AND ROOT MEAN SQUARE
C         ERRORS AND OUTPUT ERROR ANALYSIS
C
          WRITE(NWR,6400)
          EMAX=0.
          SUM=0.
          VMAX=0.
          DO 410 I=2,NFN

          YC=VEL(1)              .
          DO 411 J=1,K
  411     YC=YC*X(I)+VEL(J+1)
          VMAX=AMAX1(VMAX,ABS(YC))
          DIFF=YC-XY(I)
          IF (I-1.GT.L) GOTO 413
          WRITE(NWR,6410) I,X(I),XY(I),YC,DIFF,VEL(I-1)
          GOTO 412
  413     WRITE(NWR,6420) I,X(I),XY(I),YC,DIFF
  412     EMAX=AMAX1(EMAX,ABS(DIFF))
  410     SUM=SUM+DIFF**2
          ERMS=SQRT(SUM/FLOAT(NFN-1))
          WRITE(NWR,6430) EMAX,ERMS
          RETURN
C
 1000     GOTO (10,100,200),NDRV
C
C         FLYBACK MODE
C
  200     IF(N1.GE.3) GOTO 250
          XX=N2
          PER=PERI/4.
          IF(XX.LE.PERI/2.) GOTO 232
          XX=XX-PERI
          C1=P3-PER-XX
          S=1.
          GOTO 240
  232     C1=P3+PER-XX
          S=-1.
  240     C4=S*VMAX/PER
          V=VEL(1)*XX+VEL(2)
          IF(N1.EQ.1) RETURN
          CX=V/VMAX
          C2=S*(CX*CX-1.)
          C5=1.+P(2)*C2
          GEO=1./C5/C5
          RETURN
```

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```
C
C         DERIVATIVES
C
  250     MM=KP(1)
          IF(MM.GT.0) DF(1)=GEO
          MM=KP(2)
          IF(MM.GT.0) DF(MM)=-2.*GEO*B0*C2/C5
          IF(N1.EQ.4) RETURN
          MM=KP(3)
          IF(MM.GT.0) DF(MM)=GEO*((V/XX)*C0-B0*P(2)*V*4./C5/VMAX/PER)
          RETURN
C
C         TRIANGULAR MODE
C
   10     WRITE(NWR,6000)
          RETURN
C
C         SINE WAVE NOT AVAILABLE
C
  100     WRITE(NWR,6200)
          RETURN
C
 5000     FORMAT(80A1)
 6000     FORMAT(1H ,4X,'DRIVE MODE TRIANGULAR WAVE NOT AVAILABLE')




 6200     FORMAT(1H ,4X,'DRIVE MODE SINE WAVE NOT AVAILABLE')
 6300     FORMAT(1H ,4X,'DRIVE MODE FLYBACK WAVE')
 6400     FORMAT(1H ,//,10X,36HPOLYNOMIAL LEAST SQUARE FIT
         1ANALYSIS,//,4H   I,6X,7HX-GIVEN,7X,7HY-GIVEN,6X,
         28HY-FITTED,8X,5HERROR,10X,6HVEL(I),//)
 6410     FORMAT(1H ,I3,4X,4(1PE10.3,4X),1PE13.6)
 6420     FORMAT(1H ,I3,4X,4(1PE10.3,4X))
 6430     FORMAT(1H ,9X,5HEMAX=,1PE15.6,9X,5HERMS=,1PE15.6)
          END
```

## VITA

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In this study, a computer based Mossbauer spectrometer was built using a new MS-900 spectrometer, an Apple 2+ computer system, and a PDP 11/03 computer system. The APPLE was used as the link between the spectrometer and the PDP, which is used to analyze the Mossbauer spectra. In addition to minor hardware connections, software changes were made to the analysis program so that it could accept the data format

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produced by the new spectrometer. Due to equipment failure, only preliminary tests were made of the new system, however the tests were positive. Orginally, an Al-Fe-Ce alloy was chosen to be studied by the new system. Instead, the alloy, chosen because of its excellent high temperature properties, was studied by the original Mossbauer spectromemter system. The goal was to follow and identify changes in the microstructure of the alloy due to different processing stages. Although changes in the spectra were identified with processing stages, it is still unclear as to what compounds are related to the observed spectra.

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